An advanced real-time capable mixture controlled combustion model

Tomaž Katrašnik

University of Ljubljana, Faculty of Mechanical Engineering, Aškerčeva 6, SI-1000 Ljubljana, Slovenia, tomaz.katrasnik@fs.uni-lj.si

Abstract

The paper presents an innovative and advanced mixture controlled combustion (MCC). The MCC model is coupled to the innovative mechanistically based 0D spray model presented in a companion paper [1] that provides inputs on fuel mass distribution. Advanced MCC model is embedded into a 2-zone combustion modelling framework. Advanced MCC predicts Rate-Of-Heat-Release (ROHR) as the combination of the premixed and two diffusion parts, which correspond to rich and lean spray region. It also calculates the amount of fuel available for premixed combustion based on the duration of the ignition delay period. In addition, it reduces the reaction rate based on the oxygen availability using mechanistic basis, based on evaporation rate and based on mechanistically determined fuel amount that has reached the walls. High level of model predictability was confirmed by good agreement between the simulated and the measured ROHR traces over very broad operating range of the engine by using fixed parameters of the advanced MCC model and the spray model. Moreover, the applied modeling framework with embedded innovative spray and advanced MCC model features HiL compatible computational times.
Keywords: Diesel engine; combustion model; mixture controlled combustion; zero-dimensional; real-time compliant

Nomenclature:

$C$ model constant (-)

$d_{\text{nozzle}}$ injection nozzle diameter (m)

$F$ rate multiplication factor (-)

$H_{LHV}$ lower heating value (J/kg)

$id$ ignition delay (-)

$k$ constant in the Gaussian profile (-), turbulent kinetic energy density (m$^2$/s$^2$)

$k_A$ model constant (-)

$L_{st}$ stoichiometric air fuel ratio (-)

$\dot{M}$ momentum flux (N)

$dQ/dt$ burn rate (W)

$R$ ratio (-)

$r$ radial distance from the center line of the spray (m)

$s_{\text{tip}}$ spray tip penetration (m)

$s_1$ spray origin or tail (m)

$T$ temperature (K)

$T_A$ activation temperature (K)

$t$ time (s)

$x$ distance from the nozzle and (m)

$V$ volume (m$^3$)
\( \lambda \)  
excess air ratio (-)

\( \rho \)  
density (kg/ m\(^3\))

\( \vartheta \)  
spray cone angle (deg)

\( \tau \)  
characteristic time (s)

Subscripts and abbreviations:

\( A \)  
available

\( air \)  
air

\( B \)  
burned

\( BMEP \)  
brake mean effective pressure

\( BZ \)  
burned zone

\( comb \)  
combustion

\( CP \)  
combustion products

\( cyl \)  
cylinder

\( diff \)  
diffusive

\( EOI \)  
end of injection

\( evap \)  
everaporated

\( f \)  
fuel

\( FV \)  
fuel vapor

\( G \)  
gross

\( ign \)  
ignition

\( inj \)  
injected

\( pre \)  
premixed

\( ROHR \)  
Rate-Of-Heat-Release

\( ROI \)  
Rate-Of-Injection
1. Introduction

Global concerns on sustainable energy use and environmental protection are a continuous driving force of innovative internal combustion engine (ICE) technologies. Diesel engines feature high effective efficiency, whereas further optimization of diesel engines with the aim to increase specific power and efficiency and in particular to lower exhaust emissions is required for reaching environmental objectives and customer acceptance. One of the main scopes of this optimization is a further optimization of the combustion processes. This inherently calls for advanced and powerful simulation tools where besides the tools dedicated to detailed analyses, advanced system level tools are also of utmost importance for the virtual development process or the virtually assisted development process.

As addressed in [1], system level simulations are generally aimed to support the development process in two stages. First, system level models are indispensable for efficient exploration of the design space and pinpointing most promising design during the concept development and during the powertrain design phase. Second, efficient system engineering simulation models are also applicable as plant models for Model-in-the-Loop (MiL), Software-in-the-Loop (SiL) and Hardware-in-the-Loop (HiL) activities in the validation and calibration phase. To efficiently support these tasks system engineering simulation models
have to feature high level of accuracy and predictability as well as very fast computational times, whereas in HiL environments it is mandatory to strictly fulfil the real-time constraints [2,3].

In addition, general applicability of the models, which on one side covers the ability to model a wide range of engines and operating conditions and on the other side relates to the ability of a single model to support various stages of the development process, is of utmost importance. It reduces model calibration workload and ensures high level of consistency throughout the development process. To efficiently comply with the objectives on high level of accuracy and predictability, very fast computational times and general applicability of the models a careful selection of the appropriate physical depth of the model is required.

It was presented in [4,5] that 0D filling and emptying modeling approach with an optimized interaction of the cylinder and the gas path domains complies with the real-time constraint imposed by HiL systems on a single core processor. Furthermore, in [6] this modeling approach was extended with 2-zone combustion modeling framework presented in [7] and coupled with a MCC (mixture-controlled-combustion) model presented in [8]. It was presented in [6] that such a modelling approach also complies with a real-time constraint on a single core processor while modeling turbocharged multi-cylinder high-speed low-swept volume engine. Simulating such an engine type is demanding in terms of compliancy with the real-time constraint as small volumes call for small integration time steps and as high engine speed requires simulation of many cycles per unit of time, whereas turbocharging inherently results in more complex gas path topologies featuring large number of elements. Findings showing similar trends are also presented in [9], where authors report that a model that combines a mean-value modeling approach for the engine periphery with a 2-zone combustion modeling framework coupled with a fully empirical Vibe combustion model complies with the real-time constraint when run on a quad core processor. The latter indicates
more computational operations per engine cycle in the model presented in [9] compared to the models presented in [4,5,6].

The basic mixture controlled combustion model was presented in [10]. It relies on two hypothesis influencing the Rate-Of-Heat-Release (ROHR) calculation. First, it considers that ROHR is proportional to the fuel quantity available for combustion at the moment of consideration [10]. Second, it considers that in a Diesel engine the rate of fuel oxidation is determined by the rate of mixing of fuel vapor and fresh air/charge and thus by the local density of the turbulent kinetic energy [10]. MCC model from [10] was in [11] extended in a way that in addition to the burn rate for the diffusion part of combustion, it also addressed the ignition lag and the premixed part. The reason for this extension lies manly in the fact that in part-load conditions the premixed portion of the rate of heat release contributes significantly to the overall burn rate [11]. An additional extension of the model presented in [11], is presented in [8,12-14] where ROHR is based on the separate description of both the primary processes closely related to the fuel jet as well as the following combustion of the fuel mass remaining after the end of injection. The new features of the ROHR model prove to be necessary to describe the effects of modern high-pressure fuel injection systems on the combustion process regarding the strong influence of the injection rate on the burn rate.

Refs. [15-17] present an alternative quasi-dimensional CI model where the spray is axially discretized in slices. These slices propagate through the combustion chamber in the direction of injection and as they propagate the admixture of combustion chamber gas to the slices is stipulated by means of an empirical distribution of the excess air ratio [16]. The excess air ratio distribution of the spray has a direct impact on the diffusion combustion as the model relies on three excess air ratio zones: the extremely rich zone that is unable to burn, the zone of diffusion combustion, which also contains the stoichiometric excess air ratio, and the very lean zone [16]. The diffusion combustion considers contributions of the last two
zones, where a damping function using empirical inputs is used in [15] to account for the oxygen deficiency.

According to Ref. [15] and also according to author’s experience models that discretize the injection jet in the axial and radial direction in numerous parcels do not comply with the real-time constraint. Moreover, according to the data on computational speeds presented in [6] (that used a 0D spray model) there is also not sufficient margin in computational speed that would allow for introduction of discretized spray models while still complying with the real-time constraint. This is reasoned by two facts. First, some margin in computational speed is required to support modeling of engines with a large number of cylinders and/or with complex gas path topologies operating at high engine speed, which is of particular importance for ensuring general applicability of the models. Second, higher level of discretization inherently leads to an increased number of variables and in general also calls for smaller integration time steps as stiffness of the system commonly increases with increased spatial resolution.

To comply with the real-time requirements on computational speed of the entire engine model, an innovative 0D spray modeling framework that allows for calculation of fuel mass and mass of in-cylinder charge within selected excess air ratio limits on first principles was proposed in a companion paper [1]. The spray model is based on a non-evaporating and non-reacting spray modeling approach as mechanistic consideration of evaporation and chemical reactions inherently call for at least 1D discretization as for example presented in [18,19]. The spray model is capable of modeling the rate shaping and the spray detachment from the nozzle and allows for calculation of the fuel mass and the fraction of fuel on the wall based on first principles [1].
The innovative spray model thus provides required inputs to the presented advanced real-time capable mixture controlled combustion model with the following general features and innovative contributions:

1. ROHR prediction based on the combination of the premixed and two diffusion parts, which correspond to rich and lean spray region,
2. calculation of the fuel available for combustion based on the spray model and transport of burned fuel between the zones,
3. calculation of the fuel available for premixed combustion based on the duration of the ignition delay period,
4. mechanistically based combustion rate reduction on the oxygen availability,
5. combustion rate reduction due to evaporation,
6. rate reduction based on mechanistically determined fuel amount that has reached the walls,
7. the modeling framework is capable of considering arbitrary number of sprays.

2. Modeling framework

2.1. Interaction of the advanced MCC model with the modeling environment

The advanced (MCC) model is embedded into a 2-zone combustion modelling framework presented in [7]. The 2-zone modelling framework divides combustion chamber into a burned and unburned zone, where during the combustion mass of in-cylinder charge is transported from the unburned to the burned zone considering the combustion excess air ratio and the amount of the burned fuel given by the advanced MCC model.

The basic input on the fuel available for combustion is given by the spray model presented in [1]. Basic spray equations that are required to calculate inputs to the advanced
MCC model are recapitulated from [1] in Appendix A. The spray model relies on the input of the injection rate that is calculated by the rail model presented in [6]. As detailed hydraulic simulation models as for example [20] feature simulation times are far from real-time capability due to the detailed description of the 1D flow and the multi-body dynamics of the injection system [6], a real-time compliant 0D rail model has been proposed in [6]. In this model, the injector flow is calculated on the basis of the Bernoulli principle by modeling the nozzle flow and the needle seat throttling in two combined restrictions. The needle lift dynamics are modeled by applying force balance in the system and the opening and closing is controlled by the injection signal. A dedicated approach for consideration of pressure pulsations in the system is introduced in [6] to model pressure variation in the system.

Similar to the MCC models presented in [6,8,11-14,16,17], the advanced MCC model presented in this paper requires the input on the duration of the ignition delay period from the ignition delay model. The ignition delay model considers, similarly to the models presented in [6,8,12,14,16,17], the contribution of the Arrhenius and Magnussen terms. However, as ignition delay model is not a constitutive part of the advanced MCC model, the advanced MCC combustion model is open for integration of any ignition delay model.

All these models including the advanced MCC model are integrated in the AVL CRUISE M modeling environment presented in [4-6].

2.2. Governing equations of the advanced MCC model

2.2.1 Basic MCC ansatz

As proposed in [8,12-17], ROHR is determined as the combination of the premixed and two diffusion parts. For the purpose of the presented model ROHR is given by

\[
\frac{dQ_{comb}}{dt} = \frac{dQ_{pre}}{dt} + \frac{dQ_{diff, \lambda_{low}}}{dt} + \frac{dQ_{diff, \lambda_{hi}}}{dt} + \frac{dQ_{diff, \lambda_{R}}}{dt},
\]

(1)
where \( p_{pre} \) denotes premixed charge, \( diff, \lambda_{low} < \lambda < \lambda_{hi} \) denotes diffusion combustion within the excess air ratio limits \( \lambda_{low} \) and \( \lambda_{hi} \) and \( diff, \lambda_{hi} < \lambda < \lambda_{@R} \) denotes diffusion combustion within the excess air ratio limits \( \lambda_{hi} \) and \( \lambda_{@R} \). In this analysis results will be shown for the values \( \lambda_{low} = 0.25, \lambda_{hi} = 1.0 \), whereas \( \lambda_{@R} \) denotes the outer limit of the spray, i.e.: the boundary between the spray and the non-perturbed ambient (defining the spray radius \( R \) that corresponds to the points where the velocity is 1% of the velocity in the axis). This approach implies that the spray model from [1] is applied in a way to calculate masses within three excess air ratio regions: \( 0 < \lambda < \lambda_{low}, \lambda_{low} < \lambda < \lambda_{hi} \) and \( \lambda_{hi} < \lambda < \lambda_{@R} \), where the first one is too rich to burn and the second and the third one represent the fuel rich and lean region respectively. However, as exposed in [1] the fuel mass distribution can, due to the 0D non-evaporating and non-reacting spray modeling approach and due to the assumption \( Sc = 1 \), be to a large extent compensated by adjusting combustion limits for diffusive combustion.

For all the terms in eq. (1) it is valid

\[
\frac{dm_f}{dt} = \frac{1}{H_{LHV}} \cdot \frac{dQ}{dt},
\]

(2)

where \( H_{LHV} \) is lower heating value of the fuel.

For multiple sprays, terms of the ROHRs are summed up as

\[
\frac{dQ_{comb}}{dt} = \sum_{i=1}^{n} \left( \frac{dQ_{pre}}{dt} + \frac{dQ_{diff, \lambda_{low} < \lambda < \lambda_{hi}}}{dt} + \frac{dQ_{diff, \lambda_{hi} < \lambda < \lambda_{@R}}}{dt} \right)_{i},
\]

(3)

where \( n \) is the number of sprays. Sprays are treated independently in terms of spray propagation with the exception of the influence of the cylinder charge density that depends on the heat released by combustion. However, reaction rates of the sprays depend on the oxygen availability and thus sprays can interact in terms of reaction rate reduction as addressed in section 2.2.5. To reduce the number of indexes all derivations below are presented for a single spray without the use of spray indices.
2.2.2 Formulation of the terms in the ROHR equation

Due to extended availability of the inputs from the innovative spray model [1] advanced MCC model relies on the reformulated terms in eq. (1) given as

\[
\frac{dQ_{\text{pre}}}{dt} = C_{\text{pre}} \cdot \lambda \cdot L_{st} \cdot \frac{m_{f,U,\text{pre}A}}{V_{\text{mix}}} \cdot H_{\text{LHV}} \cdot e^{-\frac{kA}{T_A} \cdot \left(t - t_{\text{ign}}\right)^2},
\]

\[
\frac{dQ_{\text{diff},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}}{dt} = C_{\text{diff}} \cdot m_{f,U,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}A} \cdot H_{\text{LHV}} \cdot \frac{\sqrt{k}}{V_{\text{cyl}}} \cdot \left(1 - R_{f,\text{wall},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}A} \cdot (F_{\text{wall}} - 1)\right)
\]

(4)

\[
\frac{dQ_{\text{diff},\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}}}}{dt} = C_{\text{diff}} \cdot m_{f,U,\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}}A} \cdot H_{\text{LHV}} \cdot \frac{\sqrt{k}}{V_{\text{cyl}}} \cdot \left(1 - R_{f,\text{wall},\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}}} \cdot (F_{\text{wall}} - 1)\right),
\]

(5)

where \(m_{f,U,\text{pre}A}\) is the unburned fuel available for premixed combustion (section 2.2.8), \(m_{f,U,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}A}\) and \(m_{f,U,\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}}A}\) are available amounts of unburned fuel for diffusion combustion within specified lambda limits (section 2.2.9), \(C_{\text{pre}}, C_{\text{diff}}, k, T_A\) and \(F_{\text{wall}}\) are model constants, \(AF_{st}\) is stoichiometric air fuel ratio, \(t\) is current time \(t_{\text{ign}}\) is ignition timing, \(k\) is turbulent kinetic energy [10], \(V_{\text{cyl}}\) is cylinder volume, \(R_{f,\text{wall},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}A}\) and \(R_{f,\text{wall},\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}}}\) are derived in Ref. [1] (Appendix A: eq. (A7)) and

\[
V_{\text{mix}} = m_{f,\text{pre}} \cdot \left(\frac{1}{\rho_{\text{PV}}} + \frac{\lambda_{\text{pre}}L_{st}}{\rho_{\text{cyl}}}\right)
\]

(7)

where \(\rho_{\text{PV}}\) and \(\rho_{\text{cyl}}\) are density of the fuel vapor and in-cylinder charge respectively and \(\lambda_{\text{pre}}\) is the assumed lambda of the premixed combustion that is used only to calculate \(V_{\text{mix}}\).

Extensions of the advanced MCC model over the published MCC models can thus be summarized as:

a) terms \(m_{f,U,\text{pre}A}, m_{f,U,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}A}\) and \(m_{f,U,\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}}A}\) are:
- calculated by the 0D spray model based on first principles,
- limited by the evaporation rate
- limited by the oxygen availability

b) terms $R_{f,\text{wall},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}$ and $R_{f,\text{wall},\lambda_{\text{hi}}<\lambda<\lambda_{@R}}$ are calculated by the 0D spray model based on first principles.

2.2.3 Calculation of the amount of the burned fuel

Spray modeling framework presented in Ref. [1] returns as a result fuel masses within specific excess air ratio limits. However, it does not provide mass flows between these excess air ratio regions as it calculates masses based on the spray propagation determined by the momentum equation [1]. Another important aspect is also the fact that the spray model returns entire mass of the fuel within specific lambda regions, which after the start of combustion consists of unburned and burned fuel. As discernable from eqns. (4), (5) and (6), only unburned fuel is applied in calculations of the combustion rates and thus an approach for transporting burned fuel is required in the advanced MCC model. As the spray propagates, fuel is transported into regions with higher lambda values, which is also the case for the burned fuel. In the presented model, it is assumed that burned and unburned fuel is transported at the same rate. This assumption is also valid for the amount of the fuel that has reached the walls. As multiple equations in this document are equally valid for both excess air ratio regions, i.e. $\lambda_{\text{low}} < \lambda < \lambda_{\text{hi}}$ and $\lambda_{\text{hi}} < \lambda < \lambda_{@R}$, a term $x$ will be used subsequently to denote one of these regions.

At a given time $t$ the amount of fuel burned in selected lambda regions is calculated as

$$dm_{f,B,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} = \frac{1}{H_{LHV}} \cdot \frac{dQ_{\text{diff},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}}{dt} - dm_{f,B,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}<\lambda<\lambda_{@R}}$$

(8)

and
\[
dm_{f,B,\lambda_{hi}<\lambda<\lambda_{@R}} = \frac{1}{H_{LHV}} \cdot \frac{dQ_{\text{diff},\lambda_{hi}<\lambda<\lambda_{@R}}}{dt} + \dm_{f,B,\lambda_{low}<\lambda<\lambda_{hi}\rightarrow\lambda_{hi}<\lambda<\lambda_{@R}} \tag{9}
\]

where
\[
dm_{f,B,\lambda_{low}<\lambda<\lambda_{hi}\rightarrow\lambda_{hi}<\lambda<\lambda_{@R}} = \frac{m_{f,B,\lambda_{hi}<\lambda<\lambda_{@R}}}{m_{f,B,x}} \cdot \frac{\dm_{f,B,x}}{dt} \tag{10}
\]

and \(i\) and \(i-1\) represent current and previous time step thus yielding an Euler like differentiation. \(x\) in eq. (10) generally represents \(\lambda_{low} < \lambda < \lambda_{hi}\), as in the general case fuel is transported from \(\lambda_{low} < \lambda < \lambda_{hi}\) to \(\lambda_{hi} < \lambda < \lambda_{@R}\), but the solver is also capable of treating the opposite flow direction. \(\frac{dQ_{\text{diff},\lambda_{low}<\lambda<\lambda_{hi}}}{dt}\) and \(\frac{dQ_{\text{diff},\lambda_{hi}<\lambda<\lambda_{@R}}}{dt}\) in eqns. (8) and (9) respectively differ from \(\frac{dQ_{\text{diff},\lambda_{low}<\lambda<\lambda_{hi}}}{dt}\) and \(\frac{dQ_{\text{diff},\lambda_{hi}<\lambda<\lambda_{@R}}}{dt}\) (eq. (5) and (6) respectively) as both gross terms indicated by index \(G\) additionally comprise contribution of the premixed combustion as outlined in section 2.2.10.

2.2.4 Rate reduction due to evaporation

The advanced MCC model relies on the 0D non-evaporating and non-reacting spray model [1]. Therefore, evaporation is not modeled by the spray model and it thus needs to be modeled by an additional model.

There exist multiple evaporation models with various depths of details, e.g. [21-24]. 3D CFD codes generally rely on the models that calculate Sauter mean diameter and subsequent heat and mass transfer rates via correlations using non-dimensional numbers as \(\text{We}, \text{Re}, \text{Pr}, \text{Sh}\) etc. In a 0D spray model such evaporation models feature deficiencies in terms of not accurately defined local conditions, e.g. local turbulence kinetic energy and thus diffusion, local gas concentration and temperature as well local velocity difference between the droplet and the surrounding gas. Due to these deficiencies it is generally not possible to utilize such an evaporation model with fixed model parameters over a wide range of engine operating
conditions. Therefore in general more than one model parameter needs to be adjusted during the load point variation. Moreover, multiple evaporation models generally consider only one representative fuel molecule and thus such an evaporation model feature unphysically high evaporation rate when approaching critical temperature of this representative fuel molecule, which is far from the evaporation of a real D2 or similar fuel. Another deficiency of such evaporation models is their inherent requirement on short computational time steps as they incorporate exponential terms and as the evaporation rate becomes increasingly high when approaching critical temperature.

Due to the all above addressed facts a simplified evaporation model with the following ansatz function [25]
\[
\tau_{\text{evap}} = C_{\text{evap}} \cdot d_{\text{nozzle}} \cdot p_{\text{inj}}^{0.5} \cdot \rho_{\text{cyl}}^{0.3} \cdot T_{\text{cyl}}^{-3.3},
\]
has been implemented, where \(\tau_{\text{evap}}\) is the characteristic time of evaporation, \(C_{\text{evap}}\) is a single model constant, \(d_{\text{nozzle}}\) is injection nozzle diameter, \(p_{\text{inj}}\) is the injection pressure and \(\rho_{\text{cyl}}\) is the in-cylinder change density.

Unevaporated fuel \((m_{f,\text{unevap}})\) is thus balanced according to the equation
\[
dm_{f,\text{unevap}} = dm_{f,\text{inj}} - \frac{m_{f,\text{unevap}}}{\tau_{\text{evap}}} dt.
\]
where \(dm_{f,\text{inj}}\) is the injection rate and \(\frac{m_{f,\text{unevap}}}{\tau_{\text{evap}}} dt\) the rate of evaporation. Similar modeling approach with different approach to calculate \(\tau_{\text{evap}}\) is for example also given in [11].

Reduction factor \(F_{\text{evap}}\) that reduces the amount of fuel available for combustion based on the rate of evaporation is thus calculated as
\[
F_{\text{evap}} = 1 - \frac{m_{f,\text{unevap}}}{m_{f,\text{inj}}}.
\]
The reasoning for application of a simplified evaporation model models can be summarized as:

1. it allows for the use of same integration time steps as the MCC model,
2.) it has only one model, i.e. tuning, parameter,

3.) during the tests in the development and validation phase of the advanced MCC model it was shown that a single model parameters can be used over a relatively wide operating range,

4.) if 3. would not hold true for a particular engine or particular operating range of the engine, only one parameter needs to be adjusted as outlined in 2.

### 2.2.5 Rate dependency on oxygen availability

It is well known that reaction rates depend on the concentration of the reactants. On one side they are thus limited by the fuel availability, which is in the context of the proposed model accounted for via the evaporation model presented in section 2.2.4. Therefore, factors $F_{\text{diff, } \lambda_\text{low} < \lambda < \lambda_\text{hi}}$ and $F_{\text{diff, } \lambda_\text{hi} < \lambda < \lambda_@}$ that are derived in this section account for limitations due to oxygen availability, whereas combined treatment of these limiting parameters will be outlined in sections 2.2.7, 2.2.8 and 2.2.9.

$F_{\text{diff, } x}$ is determined based on the ratio of fuel and oxygen, whereas the approach is capable of treating multiple injections and thus the factor $F_{\text{diff, } x}$ is different for each spray and within a particular spray for each lambda region, i.e. $\lambda_\text{low} < \lambda < \lambda_\text{hi}$ and $\lambda_\text{hi} < \lambda < \lambda_@$.

The mass of air in the unburned zone ($UZ$) is calculated as

$$m_\text{air, } UZ = m_{UZ} \cdot \left(1 - w_{FV, UZ} - w_{CP, UZ}\right). \quad (14)$$

where $w_{FV, UZ}$ and $w_{CP, UZ}$ are the fuel vapor and combustion products concentrations in the unburned zone respectively.

The mass of combustion products for a particular lambda region is given as

$$m_{CP, x} = \left(\lambda_{BZ, x} \cdot L_{st} + 1\right) \cdot m_{f, B, x}. \quad (15)$$

where $\lambda_{BZ, x}$ is the excess air ratio of combustion products and $m_{f, B, x}$ is given by eq. (8) or (9).
The mass of air in a particular excess air ratio region is calculated as

\[ m_{\text{air},x} = (m_{\text{sp},x} - m_{f,U,x} - m_{CP,x}) \cdot R_{\text{air}}, \]  

(16)

where \( m_{\text{sp},x} \) is the mass of spray within the selected excess air ratio limits as derived in [1] (Appendix A: eq. (A5)) and \( m_{f,U,x} \) is the unburned fuel within the specified excess air ratio limits that is given as

\[ m_{f,U,x} = m_{f,x} - m_{f,B,x}, \]  

(17)

where \( m_{f,x} \) is the fuel mass within specified lambda limits as derived in [1] (Appendix A: eq. (A2)) and \( m_{f,B,x} \) is given by eqns. (8) or (9). The term \( (m_{\text{sp},x} - m_{f,U,x} - m_{CP,x}) \) thus gives the mass in a particular excess air ratio region of the spray that belongs neither to the unburned fuel nor to the combustion products. However, in general this mass does not comprise only air, which is considered by the \( R_{\text{air}} \) defined as

\[ R_{\text{air}} = \frac{m_{\text{air},UZ}}{m_{\text{cyl}} - m_{FV} - m_{CP,\lambda_{\text{low}}} < \lambda < \lambda_{\text{hi}} - m_{CP,\lambda_{\text{hi}}} < \lambda < \lambda_{@R}}. \]  

(18)

\( R_{\text{air}} \) gives the ratio between the mass of air in the unburned zone and the mass of in-cylinder charge that belongs neither to the mass of fuel vapor, i.e. unburned fuel, nor to the combustion product of both excess air ratio regions of this particular spray that are already directly accounted for in eq. (16).

Mass of air within particular lambda regions \( (m_{\text{air},x}) \) is thus derived under the assumption that each spray contains combustion products related to the burned fuel in this particular spray. However, the approach also allows for considering mixing between the sprays (which is indeed observed in the case of multiple injections) as \( R_{\text{air}} \) (eq. (18) is generally smaller than unity indicating that within the mass \( (m_{\text{sp},x} - m_{f,U,x} - m_{CP,x}) \) (eq. (16) there are in general also combustion product from other sprays. This fact also allows for plausible in-cylinder mass and volume conservation since when assuming that sprays do not
interact at all, the overall masses of multiple sprays \((m_{sp} \text{ in Ref. [1] and eq. (A6) in Appendix A})\) generally exceed the in-cylinder mass and thus also the volume.

Reduction factors \(F_{diff,x}\) that reduce reaction rate based on the availability of oxygen are thus calculated as

\[
F_{diff,x} = \frac{m_{air,x}}{l_{st} \cdot m_{f,x}}. \tag{19}
\]

2.2.6 Rate reduction due to the fuel-wall interaction

Rate reduction factors calculated in section 2.2.5 consider a free propagating spray. However, in a general case such a treatment is not fully adequate for the part of the spray that has reached the wall. After the spray has reached the wall the difference between different excess air ratio regions is less pronounced compared to the undisturbed spray. In this 0D approach, it is possible to account for this effect in a way that \(F_{diff, \lambda_{hi} \leq \lambda < \lambda_{@R}}\) (eq. (19)) is not modified, whereas \(F_{diff, \lambda_{low} < \lambda < \lambda_{hi}}\) is modified to consider that the spray can rebound from the wall or it can glide along the wall after it has reached the wall. In both cases it is generally possible to assume that fuel is mixed with air more intensively after it has reached the wall compared to the core spray region of the undisturbed spray. These ideas are summarized in the equation

\[
F_{diff, \lambda_{low} < \lambda < \lambda_{hi}, \text{wall}} = \frac{F_{diff, \lambda_{low} < \lambda < \lambda_{hi}} \cdot m_{f, \lambda_{low} < \lambda < \lambda_{hi}} + F_{diff, \lambda_{hi} < \lambda < \lambda_{@R}} \cdot m_{f, \lambda_{hi} < \lambda < \lambda_{@R}}}{m_{f, \lambda_{low} < \lambda < \lambda_{hi}} + m_{f, \lambda_{hi} < \lambda < \lambda_{@R}}}. \tag{20}
\]

Modified limiter due to the interaction of the fuel with the wall \((\tilde{F}_{diff, \lambda_{low} < \lambda < \lambda_{hi}})\) is thus calculated as

\[
\tilde{F}_{diff, \lambda_{low} < \lambda < \lambda_{hi}} = (1 - R_{f, \text{wall}, \lambda_{low} < \lambda < \lambda_{hi}}) \cdot F_{diff, \lambda_{low} < \lambda < \lambda_{hi}} + R_{f, \text{wall}, \lambda_{low} < \lambda < \lambda_{hi}} \cdot F_{diff, \lambda_{low} < \lambda < \lambda_{hi, \text{wall}}}. \tag{21}
\]
which transforms from $F_{\text{diff}, \lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} \text{ to } F_{\text{diff}, \lambda_{\text{aiw}}<\lambda<\lambda_{\text{hi,wall}}}$ based on the $R_{f, \text{wall}, \lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}$, which gives the amount of the fuel that has hit the wall [1] (Appendix A: eq. (A7)).

If it is assumed that most of the fuel sticks onto the wall and thus that the fuel is not mixed with air more intensively after it has reached the wall, eq. (19) can be used in its original form and $F_{\text{diff}, \lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}$ is valid for the entire combustion period.

### 2.2.7 Evaluation of the fuel available for combustion

As addressed in sections 2.2.3, 2.2.4 and 2.2.5 all the fuel that is mixed above $\lambda_{\text{low}}$, i.e. $m_{f, \lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}$ and $m_{f, \lambda_{\text{hi}}<\lambda<\lambda_{\@R}}$ from Ref. [1] (Appendix A: eq. (A2)), is not available for combustion as some of this fuel can already be burned (section 2.2.3 and 2.2.5), some of the fuel might not yet be evaporated (section 2.2.4) and reaction rates in specific regions can be reduced due to the limited availability of oxygen (section 2.2.5). Evaluation of available unburned fuel within specified lambda limits is given in eq. (17), whereas after consideration of evaporation rate and oxygen availability gross available (GA) amount of unburned fuel within specified lambda limits is given as

$$m_{f, U, \lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}, \lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}, \text{GA} = m_{f, U, \lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}, \lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}, \text{GA} + m_{f, U, \lambda_{\text{hi}}<\lambda<\lambda_{\@R}, \lambda_{\text{hi}}<\lambda<\lambda_{\@R}}, \text{GA}.$$  (23)

### 2.2.8 Evaluation of the fuel available for premixed combustion
It is well known that a certain amount of fuel burns in a premixed phase of the Diesel combustion. However, spray model presented in [1] (and also other spray models) does not separately predicts the premixed fuel quantity as this quantity is mainly determined by the duration of the ignition delay period and not the spray dynamics. Therefore the amount of the fuel that burns in the premixed phase is considered to be a part of the fuel that has mixed above $\lambda_{low}$, i.e. $m_{f,\lambda_{low}<\lambda<\lambda_{hi}}$ and $m_{f,\lambda_{hi}<\lambda<\lambda_{R}}$, which is indeed resembles the real process in the engine. To increase the level of predictability of the model, presented model assumes linear increase of the share of the fuel that is burned in the premixed phase ($R_{pre}$) with the ignition delay given as

$$R_{pre} = A_{pre} + B_{pre} \cdot t_{id},$$

(24)

where $A_{pre}$ and $B_{pre}$ are model constants and $t_{id}$ is the ignition delay period given in time basis.

With the use of eq. (24) the available amount of the fuel that will burn as the premixed fuel is calculated as

$$m_{f,pre,A} = R_{pre} \cdot m_{f,inj} \big|_{t_{ign}},$$

(25)

where $m_{f,inj} \big|_{t_{ign}}$ represents amount of injected fuel at ignition or start of combustion.

With this input available amount of unburned fuel for premixed combustion is calculated as

$$m_{f,U,pre,A} = m_{f,pre,A} - m_{f,B,pre},$$

(26)

where $m_{f,B,pre}$ denotes fuel burned in the premixed combustion, which is given by combining eq. (4) and eq. (2).

2.2.9 Evaluation of fuel available for diffusion combustion
As discernable from section 2.2.8 the premixed combustion sources fuel from the excess air ratio regions \( \lambda_{\text{low}} < \lambda < \lambda_{\text{hi}} \) and \( \lambda_{\text{hi}} < \lambda < \lambda_{\text{R}} \). Therefore, notation “gross available amount of unburned fuel within selected excess air ratio limits” was used for \( m_{f,U,X,GA} \) in eq. (22) as it comprises fuel for diffusive and also for the premixed combustion. This section thus outlines the evaluation of the available amount of unburned fuel within the selected excess air ratio limits \( (m_{f,U,X,A}) \), which does not comprise the amount available for premixed combustion. It is assumed that the amount of premixed fuel is taken from the \( m_{f,U,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}},GA} \) and \( m_{f,U,\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}},GA} \) in proportional amounts and thus

\[
m_{f,U,X,A} = F_{\text{pre}} \cdot m_{f,U,X,GA},
\]

(27)

where

\[
F_{\text{pre}} = 1 - \frac{m_{f,U,\text{pre},A}}{m_{f,U,A}}
\]

(28)
gives the ratio between available amount of unburned fuel within both excess air ratio regions and the available amount of fuel for combustion.

2.2.10 Evaluation of the gross diffusion combustion rates

As the premixed combustion sources fuel from the \( m_{f,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}},GA} \) and \( m_{f,\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}},GA} \) (section 2.2.8), it is also necessary to consider the fuel burned in the premixed phase when evaluating the amounts of the burned fuel in the diffusion combustion (section 2.2.3), which in turn defines the amounts of the unburned fuel (section 2.2.5). The fuel for premixed combustion is taken from \( m_{f,U,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}},GA} \) and \( m_{f,U,\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}},GA} \) in proportional amounts and thus \( \frac{dQ_{\text{pre}}}{dt} \) from eq. (4) is also added to \( \frac{dQ_{\text{diff},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}}}{dt} \) and \( \frac{dQ_{\text{diff},\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}}}}{dt} \) (in eqns. (5) and (6) respectively) in proportional amounts to calculate \( \frac{dQ_{\text{diff},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}},G}}{dt} \) and

\[
\frac{dQ_{\text{diff},\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}},G}}{dt}
\]

used in eqns. (8) or (9) as
\[
\frac{dQ_{\text{diff} \lambda_{\text{low}} < \lambda < \lambda_{\text{hi}}}}{dt} = \frac{dQ_{\text{diff} \lambda_{\text{low}} < \lambda < \lambda_{\text{hi}}}}{dt} + \frac{m_{f, U, \lambda_{\text{low}} < \lambda < \lambda_{\text{hi}}}}{m_{f, U, GA}} \cdot \frac{dQ_{\text{pre}}}{dt},
\]

and

\[
\frac{dQ_{\text{diff} \lambda_{\text{hi}} < \lambda < \lambda_{\text{R}}}}{dt} = \frac{dQ_{\text{diff} \lambda_{\text{hi}} < \lambda < \lambda_{\text{R}}}}{dt} + \frac{m_{f, U, \lambda_{\text{hi}} < \lambda < \lambda_{\text{R}}}}{m_{f, U, GA}} \cdot \frac{dQ_{\text{pre}}}{dt},
\]

where distribution \( \frac{dQ_{\text{pre}}}{dt} \) is done according to eq. (28).

### 3. Results

In this section a low and a high engine operating load points are analyzed in more detail first to provide insight into the modeling approach, whereas afterwards ROHR curves along with the Rate-Of-Injection (ROI) curves are shown to further validate the model. Results are shown for a 5-cylinder turbocharged Diesel AVL research engine with high pressure EGR, charge air cooler and a common rail injection system. The engine parameters are given in Table 1. The engine is equipped with high pressure indication and detailed injection system measurement instrumentation. Therefore, in addition to the measured crank-angle resolved in-cylinder pressure trace also the data of crank-angle resolved needle lift and injector pipe pressure are available. During the model preparation phase the model of the engine gas path and the rail model were calibrated in a way to ensure good agreement between measured and simulated parameters in the engine manifolds, which ensure adequate boundary conditions for simulating the in-cylinder processes and thus for the combustion model.

It is important to note that all results shown in this section are calculated with fixed parameters of the advanced MCC model and the spray model, i.e. all equations presented in section 2.2 of this paper and all spray equations from Ref. [1] have fixed model parameters and are not subjected to any point-to-point tuning. Parameters of the advanced MCC model that are applied in the presented analysis are listed in Appendix B. These parameters were...
determined manually, whereas, if required, approaches featuring higher level of automatism, e.g. [11], can be applied to determine model parameters. Unlike the parameters of the combustion model, the parameters of the ignition delay model presented in section 2.1 (which is not a constitutive part of the combustion model as the advanced MCC combustion model is open for integration of any ignition delay model) do need to be adjusted in certain operating points to accurately predict the start of combustion.

3.1. High load operating point

In this section results are shown for a relatively high load engine operating point characterized by 14.1 bar BMEP @ 3400 rpm, average injection pressure of approx. 1400 bar and injected fuel quantity per cylinder per cycle of approx. 41 mg. As already discussed in [1], Figure 1a shows that $m_{f,0<\lambda<0.25}$ increases immediately after start of injection (SOI) for the injection profile given in Figure 1d, whereas $m_{f,0.25<\lambda<1}$ and $m_{f,1<\lambda<\lambda_R}$ increase with some delay as the spray tip penetrates further into the combustion chamber. Moreover, it can be seen that after the end of injection (EOI shown in Figure 1d and indicated by the point where $m_{f,inj}$ reaches its maximum value) $m_{f,0<\lambda<\lambda_{low}}$ drops to zero as the consequence of the spray dynamics and thus due to air or in-cylinder charge entrainment into the spray. Similarly, also $m_{f,0.25<\lambda<1}$ decreases and thus with prolonged time after EOI all the fuel is gradually mixed with the air or in-cylinder charge above $\lambda = 1$.

Figure 1b shows masses of available amounts of unburned fuel for premixed combustion and both diffusion combustion contributions. It can be seen that values of of $m_{f,U,pre,A}$, $m_{f,U,0.25<\lambda<1,A}$ and $m_{f,U,1<\lambda<\lambda_R,A}$ are much lower compared to the masses shown in Figure 1a, as some of the fuel injected after SOI and in the early stage of combustion has not yet
evaporated (section 2.2.4), some of the fuel has already burned and available amounts of unburned fuels can additionally be reduced due to potential oxygen deficiency (section 2.2.5).

As \( m_{f,U,pre,A} \), \( m_{f,U,0.25<\lambda<1,A} \) and \( m_{f,U,1<\lambda<\lambda_{b@R,A}} \) present inputs in equations for evaluation of premixed and diffusion combustion, i.e. eqns. (4), (5) and (6) respectively, trends of \( \frac{dQ_{pre}}{dt} \), \( \frac{dQ_{diff,0.25<\lambda<1}}{dt} \) and \( \frac{dQ_{diff,1<\lambda<\lambda_{b@R}}}{dt} \) in Figure 1c resemble the ones of \( m_{f,U,pre,A} \), \( m_{f,U,0.25<\lambda<1,A} \) and \( m_{f,U,1<\lambda<\lambda_{b@R,A}} \) in Figure 1b. However, the ratios among \( \frac{dQ_{pre}}{dt} \), 

\[
\frac{dQ_{diff,0.25<\lambda<1}}{dt} \quad \text{and} \quad \frac{dQ_{diff,1<\lambda<\lambda_{b@R}}}{dt}
\]
do not match those of \( m_{f,U,pre,A} \), \( m_{f,U,0.25<\lambda<1,A} \) and \( m_{f,U,1<\lambda<\lambda_{b@R,A}} \) due to the formulation of the burn rate equations (eqns. (4), (5) and (6)).

Figure 1d thus shows that both simulated ROI an ROHR match very well the experimental ROI and ROHR. ROI model [6] provides input to the spray model (presented in [1]) providing input for the advanced MCC combustion model yielding the simulated ROHR as an output. Good agreement between the simulated and the experimental ROI confirms prediction capability of the rail model [6], whereas good agreement between the simulated and the experimental ROHR traces confirms the capability of the spray model (that is already separately validated in [1]) and the advanced MCC model to predict ROHR trace with high accuracy.

### 3.2. Low load operating point

The second analyzed point features a relatively low load engine operating point characterized by 6.9 bar BMEP @ 1800 rpm, average injection pressure of approx. 800 bar and injected fuel quantity per cylinder per cycle of approx. 20 mg. Figure 2a again shows the traces of fuel masses, which highlight mixing of the fuel into regions with higher excess air ratio values.
Figure 2b clearly indicates a longer ignition delay period being indicated by the longer period from the SOI in Figure 2d and availability of the fuel for premixed combustion \( (m_{f,U,pre,A} > 0) \), which is, as presented in section 2.2.8, initiated at the start of combustion. The longer ignition delay period in this operating point is explained by the lower injection pressure and the lower in-cylinder temperature and pressure which come as the consequence of the lower engine load compared to the operating point analyzed in section 3.1. Consequently, more fuel is available for premixed combustion as presented in section 2.2.8 resulting in very pronounced premixed combustion rate shown in Figure 2c.

This is also clearly discernable in Figure 2d, which shows a pronounced peak of premixed combustion being characteristic for low load operation. In addition, Figure 2d again confirms good agreement between simulated and measured ROI and ROHR traces further proving credibility of the spray and the combustion model.

### 3.3. Additional operating points

Figure 3 shows additional operating points that indicate good agreement between simulated and measured ROI and ROHR traces over a very broad operating range of the engine. When assessing these figures it is important to again note that all results shown are calculated with fixed parameters of the advanced MCC model and the spray model, which proves high predictability of the modeling framework over a very broad operating range of the engine. It is certainly possible to further tune the models to push the agreement between the simulation and the experiment to within the line thickness, however this is much less important compared to confirming the high level of predictability of the modeling framework using fixed model parameters. This high level of predictability namely qualifies this model suitable for application in early development stages, for parametric studies and for late
calibration and validation stages of the development where the model has to respond plausibly to varying controller parameters.

3.4. Computational speed

Both the spray and the advanced MCC model were in addition to considering plausible modeling basis developed with the aim to ensure real-time computational times. Real-time factors of the entire engine model including the gas path thus range from 0.4 up to 0.65 for the analyzed operating points presented in this section on a single core of a 2.5 GHz processor. These computational times coincide well with the computational times given in [6], where the MCC model presented in [8] was integrated in the same engine and gas path modeling framework as used in the presented analysis [4,7]. This indicates that the advanced MCC model and the innovative spray model [1] features similar computational expenses to the MCC model presented in [8]. In addition, it is demonstrated in [4] that the applied modeling framework of the entire engine allows achieving nearly constant real-time profile over the computational time, which is also valid for embedded 2-zone combustion modeling framework [7] as presented in [6]. It can thus be concluded that the proposed advanced MCC model and the innovative spray model [1] that are embedded in an engine modeling framework [4,7] comply with the real-time constraints imposed by the HiL systems for engine models of high-speed low-swept volume engines.

4. Conclusions

An innovative and advanced MCC model is presented in the paper. The MCC model is coupled to the innovative mechanistically based 0D spray model presented in a companion paper [1]. The entire chain of models - from the ROI (being the input to the spray model)
over models for calculating available unburned fuel for combustion to the calculation of the combustion rates - was developed either on a mechanistic basis or by considering the most influencing phenomena when developing the ansatz functions of the model. As a result the model features a very high level of predictability of the entire modeling framework using ROI as an input and returning ROHR as the results. This high level of predictability was confirmed by the good agreement between the simulated and measured ROHR traces over very broad operating range of the engine by using fixed parameters of the advanced MCC model and the spray model. Moreover, the applied modeling framework with embedded innovative spray and advanced MCC model features real-time factors significantly below unity on a single core for all the analyzed points making it HiL compatible.

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Appendix A

Appendix A summarizes basic spray equations that are derived in [1]. Equations are given without the detailed derivations that are in its full form presented in [1] and are thus intended to ensure integrity of the paper and to provide basic information to the reader.

Fuel mass in the region from the spray core up to a selected excess air ratio $\lambda_1$ is calculated as

$$m_{f, 0 < \lambda < \lambda_1} = \frac{\pi \rho}{2k \hat{M}} \cdot \hat{m}_f \cdot \tan \left( \frac{\theta}{2} \right) \cdot \left( s_{\lambda_1, \text{max}}^3 - s_{\lambda_1, \text{min}}^3 \right) - \frac{\pi \rho}{3k} \cdot \tan^2 \left( \frac{\theta}{2} \right) \cdot \frac{1}{1 + \lambda_1 \cdot L_{st}} \cdot$$

$$\left( s_{\lambda_1, \text{max}}^3 - s_{\lambda_1, \text{min}}^3 \right),$$

(A1)

where $\rho$ is density of the spray, $k$ constant in the Gaussian profile, $\hat{M}$ time averaged momentum flux, $\hat{m}_f$ time averaged fuel flow, $\theta$ spray cone angle, $s_{\lambda_1, \text{min}}$ and $s_{\lambda_1, \text{max}}$ are lower and upper integral boundaries considering spray dynamics and fuel concentration.
distribution. Fuel mass between selected excess air ratio limits \( \lambda_1 \) and \( \lambda_2 \), where \( \lambda_2 > \lambda_1 \), is thus calculated as

\[
m_{f, \lambda_1 < \lambda < \lambda_2} = m_{f, \lambda_0 < \lambda < \lambda_2} - m_{f, \lambda_0 < \lambda < \lambda_1}.
\]  \( \text{(A2)} \)

Spray mass in the region from the spray core up to a selected excess air ratio \( \lambda_1 \) is calculated as

\[
m_{sp, \lambda_0 < \lambda < \lambda_1} = -\frac{\pi \cdot \rho \cdot \tan^2 \left( \frac{\theta}{2} \right)}{3 \cdot k} \cdot \left[ s_{\lambda_1, max} \cdot \left( \ln (s_{\lambda_1, max} \cdot A) - \frac{1}{3} \right) - s_{\lambda_1, min} \cdot \left( \ln (s_{\lambda_1, min} \cdot A) - \frac{1}{3} \right) \right].
\]  \( \text{(A3)} \)

where

\[
A = \frac{\tan \left( \frac{\theta}{2} \right)}{\sqrt{\pi \cdot \rho \cdot \tilde{m}_f \cdot (1 + \lambda_1 \cdot L_{st})}}
\]  \( \text{(A4)} \)

Again spray mass between selected excess air ratio limits \( \lambda_1 \) and \( \lambda_2 \), where \( \lambda_2 > \lambda_1 \), is calculated as

\[
m_{sp, \lambda_1 < \lambda < \lambda_2} = m_{sp, \lambda_0 < \lambda < \lambda_2} - m_{sp, \lambda_0 < \lambda < \lambda_1}.
\]  \( \text{(A5)} \)

Total spray mass \( (m_{sp}) \) is calculated as

\[
m_{sp} = 2 \cdot \pi \cdot \rho \cdot \int_{s_1}^{s_{tip}} \int_0^R r \cdot dr \cdot dx = \frac{\pi \cdot \rho \cdot \tan^2 \left( \frac{\theta}{2} \right)}{3} \cdot \left( s_{tip}^3 - s_1^3 \right)
\]  \( \text{(A6)} \)

where \( s_{tip} \) is spray tip penetration and \( s_1 \) denotes spray origin or tail.

Ratios of the fuel masses on the wall to the fuel mass within arbitrary excess air ratio limits as for example given for excess air ratio limits \( \lambda_1 \) and \( \lambda_2 \) is calculated as

\[
R_{f, wall, \lambda_1 < \lambda < \lambda_2} = \frac{m_{f, wall, \lambda_1 < \lambda < \lambda_2}}{m_{f, \lambda_1 < \lambda < \lambda_2}},
\]  \( \text{(A7)} \)

where \( m_{f, \lambda_1 < \lambda < \lambda_2} \) is given by eq. (A2) and \( m_{f, wall, \lambda_1 < \lambda < \lambda_2} \) represents the fuel mass that has reached the wall as derived in [1].
Appendix B

Table 2 summarizes parameters of the advanced MCC combustion model. All results presented in the paper are calculated with fixed parameters of the advanced MCC model and the spray model.

![Graph a)](image1)

![Graph b)](image2)
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Figure 1 a) Time evolution of the injected fuel ($m_f$) and masses of fuel within selected excess air ratio limits, b) masses of fuel available for combustion and mass of unevaporated fuel, c) reaction rates of premixed and both diffusion combustion contributions, and d) comparison of simulated and experimental ROI and ROHR traces.
Figure 2 a) Time evolution of the injected fuel ($m_f$) and masses of fuel within selected excess air ratio limits, b) masses of fuel available for combustion and mass of unevaporated fuel, c) reaction rates of premixed and both diffusion combustion contributions, and d) comparison of simulated and experimental ROI and ROHR traces.
Figure 3 Comparison of simulated and experimental ROI and ROHR traces for operating points: a) 1.8 bar BMEP @ 1400 rpm, b) 5.9 bar BMEP @ 3400 rpm, c) 11.2 bar BMEP @ 2600 rpm, and d) 14.3 bar BMEP @ 1800 rpm

Table 1 Parameters of the analyzed engine.

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<tr>
<td>EGR Rate</td>
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<tr>
<td>Swirl (AVL nomenclature)</td>
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<td>0.4 -1.4 [bar rel.]</td>
</tr>
<tr>
<td>Injection System</td>
<td>Common Rail</td>
</tr>
<tr>
<td>parameter</td>
<td>equation</td>
</tr>
<tr>
<td>-------------------</td>
<td>----------------</td>
</tr>
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<td>$k_A \cdot T_A$</td>
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<td>$C_{diff}$</td>
<td>eq. (5) and (6)</td>
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<td>$F_{wall}$</td>
<td>eq. (5) and (6)</td>
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Table 2 Parameters of the combustion model.
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<tr>
<td>$B_{pre}$</td>
<td>eq. (24)</td>
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<td>[s$^{-1}$]</td>
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