Innovative 0D transient momentum based spray model for real-time simulations of CI engines

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Abstract

The paper presents an innovative mechanistically based spray model intended for use in mixture-controlled-combustion models. The primary objective of the spray model is to predict masses of fuel within selected limits of excess air ratios during and after the end of injection. The model is based on a 0D non-vaporizing and non-reacting modelling framework to ensure short computational times. These assumptions represent clear simplifications compared to the real transient spray propagation phenomena in reacting turbulent flows. However, from the study, it is concluded that the modelling framework is capable of attaining an adequate level of predictability for system-level applications. The model is capable of predicting spray detachment from the nozzle after the end of injection. This feature is crucial for plausible prediction of masses within selected excess air ratios. The spray model is also capable of determining the fuel mass reaching the wall. In addition, the spray modelling framework is capable of considering injection rate-shaping and evaluating its impact on predicted masses of fuel within selected limits of excess air ratios. The spray model is successfully validated against experimental data for varying injection parameters and ambient densities, demonstrating its reliability and applicability.

Keywords: spray model; Diesel engine; zero-dimensional; mechanistically based; real-time compliant

Nomenclature:

\[ A \quad \text{cross section (m}^2) \]
Fuel concentration (-)

Mass fraction of the fuel vapour (-)

Constant in the Gaussian profile (-)

Stoichiometric air fuel ratio (-)

Momentum (Ns)

Momentum flux (N)

Mass (kg)

Mass flow (kg/s)

Spray radius (m)

Ratio of the fuel mass that has reached the wall to the fuel mass (-)

Distance between the wall and the injector hole (m)

Radial distance from the centreline of the spray (m)

Spray tip penetration (m)

Spray origin or tail (m)

Schmidt number (-)

Time (s)

Velocity (m/s)

Volume (m$^3$)

Distance from the nozzle exit (m)

Spray cone angle (deg)

Excess air ratio (-)

Density (kg/ m$^3$)

Subscripts and abbreviations:

$a$  
air

cg  
centre of gravity

cl  
centreline

$CV$  
control volume

cyl  
cylinder

$f$  
fuel

$inj$  
injected

$l$  
liquid
**1. Introduction**

Global concerns in the areas of sustainable energy use and environmental protection are a continuous driving force for innovative internal combustion engine (ICE) technologies. One of the criteria for achieving environmental objectives and customer acceptance is further optimization of Diesel engines with the aim to achieve high specific power and fuel efficiency at low exhaust emissions. These objectives motivate the development of advanced and powerful simulation tools that efficiently support the virtual development process.

System-level simulations are generally implemented to support the development process in two stages. First, system-level models are indispensable for efficient exploration of the design space and identification of the most promising designs during the concept development and powertrain design phases. Second, efficient system engineering simulation models are used 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 phases. To support these tasks, system engineering simulation models require fast computational times, whereas in HiL environments it is mandatory to strictly fulfil the real-time constraints as presented by Pfau et al. [1] and Katrašnik et al. [2]. In addition to computational speed, accuracy and predictability are of significant importance for general applicability of system-level simulation models.

To preserve a high level of consistency throughout various stages of the development process and to reduce model calibration workload, it is beneficial to use consistent plant models over the complete development process. Therefore, a careful selection of the appropriate physical depth of the model is required to efficiently fulfil the objectives concerning computational speed, accuracy and predictability. It was reported by Wurzenberger et al. [3,4] that the 0D filling and emptying modelling approach, with an optimized interaction of the cylinder and the gas path domains, complies with the real-time constraints imposed by HiL systems on a single core processor. Moreover, Poetsch [5] noted that an extension of this modelling approach with a two-zone combustion modelling framework coupled with a mixture-controlled-combustion (MCC) model presented by Pirker
at al. [6] also complies with the real-time constraints on a single core processor. Maroteaux et al. [7] presented a model that combined a mean-value modelling approach for the engine periphery with a two-zone combustion modelling framework relying on an empirical combustion model. They reported that the model complied with the real-time constraint when run on a quad core processor [7]. The need to use a quad core processor to comply with the real-time constraint implies more computational operations per engine cycle in the model presented in [7] compared to the models presented in [3-5].

The basic mixture-controlled combustion model presented by Chmela et al. [8] relies on the assumption that the rate of heat release (ROHR) of a CI engine is controlled primarily by the instantaneous fuel mass present in the in-cylinder charge and the local density of turbulent kinetic energy. This modelling approach was extended by Chmela et al. [9] to incorporate premixed combustion. Refs. [6,10-12] present additional extensions of the modelling approach to distinguish between jet combustion and the burn-out phase of diffusion combustion. Additionally, Refs. [13-15] present a quasi-dimensional CI model in which spray is axially discretized in slices and a probability density function is used in the radial direction to divide the slice into the rich, stoichiometric and lean regions. ROHR is again obtained as the sum of the premixed contribution and two diffusion contributions per spray, whereas a damping function using empirical inputs is used by Grill et al. [13] to account for oxygen deficiency.

Grill et al. [13] additionally noted that it is important to model the influence of injection rate on the burn rate. This is not possible with the spray model used in the MCC model outlined in Refs. [6,10-12], which is based on the spray modelling approach proposed by Garcia Oliver [16] and Lopez Sanchez [17]. Spray models in [16,17] and also in [18,19] were derived for a constant momentum in-flux (i.e., a constant velocity at the nozzle) as well as constant ambient conditions.

According to Ref. [13], models that discretize the injection jet into numerous packages in the axial and radial direction do not comply with the real-time constraint. Moreover, according to the data on computational speeds of the model presented in [5] (which used a 0D spray model), there is also an insufficient margin in computational speed that would allow for introduction of discretized spray models while still complying with the real-time constraint. This conclusion is based on the following two points. First, some margin in computational speed is required to support modelling of engines with a large number of cylinders and/or complex gas path topologies operating at high engine speed, which is of particular
importance for ensuring general applicability of the models. Second, a higher level of
discretization inherently leads to an increased number of variables and generally implies
smaller integration time steps, as the stiffness of the system typically increases with
increasing spatial resolution. The use of 0D modelling depth implies a non-vaporizing and
non-reacting spray modelling approach, as mechanistic consideration of evaporation and
chemical reactions inherently call for at least 1D discretization, as illustrated by studies by
Pastor et al. [20] and Desantes et al. [21].

This paper thus focuses on an innovative and computationally efficient 0D spray model
intended for use in real-time-capable MCC models, as presented by Katrašnik [22]. The main
objective of the spray model is thus to predict masses of fuel within selected limits of excess
air ratios during and after the end of injection that are required by the combustion model. To
comply with the above requirements, the spray model is based on the transient momentum
equation solved in 0D and incorporating non-vaporizing and non-reacting assumptions, as
well as Gaussian distributions, of spray velocity and fuel concentration around the centreline.

2. Analytical Framework

A schematic of the spray geometry with nozzle indicated is presented in Figure 1. The
time-dependent rate of injection represents an input to the spray model. According to the
basic assumption of non-vaporizing sprays, no specific distinction is made between the fuel
in the liquid or vapour state. The momentum flux of the fuel through the nozzle is thus
calculated for the liquid fuel, whereas immediately from the onset of the conical spray region
a gas jet is assumed, as reasoned in Ref. [18], and thus the fuel is treated as fuel vapour
thereby neglecting fuel evaporation and associated phenomena (a more detailed description is
given in section 2.10). This approach is supported by the findings of Ricou and Spalding [23]
indicating that different gas jets behave in a similar way if momentum and exit velocity are
the same, which also forms the basis for applying the equivalent diameter approach to spray
modelling as presented in Ref. [18], for example. The spray mass consists of the injected fuel
in the vapour phase and the entrained in-cylinder charge. The density in the spray is thus
calculated assuming properties of the fuel in the vapour phase and properties of the entrained
in-cylinder charge as outlined in section 2.8, whereas excess air ratio is calculated from the
known fuel concentration.

In addition to the 0D spatial resolution and non-vaporizing and non-reacting modelling
approach, basic assumptions of the model can be summarized as follows:
1. At any distance from the nozzle, the spray velocity exhibits a Gaussian distribution around the centreline as outlined in, e.g., [20].
2. At any distance from the nozzle, the fuel concentration exhibits a Gaussian distribution around the centreline as outlined in, e.g., [20].
3. The Schmidt number, $Sc$, is assumed to be equal to 1.
4. The density of the entire spray is spatially constant but changes with time.
5. The spray features a constant spray cone angle.
6. The spray model is based on the convection-driven momentum equation, in which diffusion, surface and volume sources are not modelled directly, with the former two considered via assumptions 1 and 2.
7. The momentum in-flux is only through the fuel injected from the nozzle.
8. The velocity at the nozzle exit is uniform.
9. The spray is circumferentially symmetrical along the axis of the nozzle.

Compared to detailed and thus computationally demanding spray models, e.g., Vujanović et al. [24], Xiao et al. [25] and Perini et al. [26], multiple physicochemical phenomena such as atomization, drop breakup/coalescence, drop drag, evaporation, chemical kinetics and physics-based modelling of turbulence, diffusion and wall impingement are not taken into account in the proposed simplified spray modelling approach. Therefore, before analysing the implications of the listed assumptions, it is worth repeating that the spray model is intended for use in a real-time-capable advanced MCC model, in which real-time compliancy should be ensured for the model of the entire engine.

Assumptions of non-vaporizing and non-reacting spray thus neglect temperature, pressure and compositional variations caused by evaporation and chemical reactions. These two simplifications influence the density distribution [20,21] and thus the spray angle at a certain distance from the nozzle [21]. However, [20,21] also indicate that the velocity at the centreline is not affected significantly if both effects are neglected. This conclusion can, to a large extent, be transferred also to prediction of the spray tip penetration and thus to prediction of masses of fuel within the selected limits of excess air ratios, as they are mostly influenced by the velocity at the centreline and the spray angle. In addition, Payri et al. [27] concluded that the spray contours of the reacting spray and inert spray do not differ significantly and that the difference is relatively small up to the penetration distances being in the range of the spray free path in the high-speed Diesel engines.
Similarly, Nabers et al. [28] reported that evaporation decreases the spray cone angle and the spray tip penetration compared to the non-vaporizing conditions. However, they concluded that the differences decrease for the higher ambient densities that are generally encountered during injection in modern Diesel engines. This finding can be used to justify assumption 5 of the constant spray cone angle, which should be considered in light of the objective of the spray model being the prediction of the masses of fuel within selected limits of excess air ratios at the system level. Furthermore, Nabers et al. [28] and Klein-Douwel et al. [29] noted that the spray angle also varies during a single injection period with the largest variation during the early injection period, which is less relevant for masses of fuel within the excess air ratios relevant for combustion.

A non-vaporizing and non-reacting assumption should also be considered along with the assumption of the Gaussian velocity and fuel concentration distributions (assumption 1 and 2) being additionally influenced by assumptions 6 and 7. The Gaussian distribution covers all interactions of the spray with its surroundings including entrainment of the in-cylinder charge. It thus, in combination with conical spray propagation, accounts for radial spray propagation and all associated transport phenomena, including turbulence and diffusion. Although the assumption of Gaussian distribution is well supported by experimental data, e.g., [30] for the steady state condition, its validity is less certain for the transient calculations of spray front penetration. The self-similarity of the profile can thus be assumed for the steady state condition, whereas curvature of the transient spray front can be larger as the velocity approaches zero at $R(x)$ (Figure 1), and thus the difference between the velocity at the spray tip and at the spray boundaries can be larger for the transient spray.

The potential error introduced by $Sc = 1$ (assumption 3), which implies similarity between the transport of momentum and the transport of mass, should also be considered along with previous assumptions, which introduce a certain error in comparison to real phenomena in turbulent, vaporizing and reactive sprays. In addition, Ref. [19] reports that variations of $Sc$ do not significantly influence the spray tip velocity and consequently the spray tip penetration as well as masses of fuel within the selected limits of excess air ratios. It is worth noting that potential errors in fuel mass distribution from the assumption of $Sc = 1$ can be compensated by adjusting combustion limits in the diffusive combustion model as, for example, presented in [22].

The assumption of spatially constant spray density (assumption 4) is required to ensure an analytic solution of the governing equations, outlined in section 2.1, which is a prerequisite
for fast computation. This assumption influences the evaluation accuracy of the spray dynamics; however, as reported in [18], it is possible to obtain satisfactory results describing spray tip penetration using the assumption of spatially constant spray density. Despite the fact that local spray density, which exhibits large variations, is not evaluated properly as a result of this assumption, it is possible to satisfactorily model spray tip penetration under the assumption of constant spray density [18]. This is an important fact, as in the 0D model the spray tip penetration significantly influences determination of the masses of fuel within the selected limits of excess air ratios, which is the main objective of the proposed spray model.

In addition, the convection-driven momentum equation in assumption 6 ignores pressure gradients and thus delays in information propagation. Neglecting delays in information propagation might be justified for the liquid core of the spray because of the low compressibility of the liquid and its high propagation velocities, but it certainly leads to some discrepancies compared to the phenomena in peripheral parts of sprays with high gas content because of their higher compressibility and lower propagation velocities.

The boundary condition on the uniform velocity profile at the nozzle (assumption 8) is commonly used in analyses in which detailed boundary conditions of the two-phase spatially inhomogeneous outflow from the nozzle are not available or cannot be considered, e.g., [18-20,28].

Circumferential symmetry of the spray along the axis of the nozzle (assumption 9) is a valid assumption for low-swirl engines. Therefore, the derived equations assume that the impact of the swirl on the spray tip penetration and the circumferential distribution is sufficiently small to allow for plausible evaluation of the masses of fuel within selected limits of excess air ratios. These last four assumptions also need to be assessed under consideration of the objective on the spray model (i.e., prediction of the masses of fuel within selected limits of excess air ratios), in which potential errors in fuel mass distribution can be compensated by adjusting combustion limits in the diffusive combustion model as, for example, presented in [22].

It can thus be concluded that the assumptions introduce deviations from the real phenomena of vaporizing and reactive sprays. However, when considering the intended application of the spray model being aimed to provide input data to the real-time-capable advanced MCC model, it can be concluded that deviations of the spray model are in comparable range to those imposed by the 0D modelling depth of the in-cylinder processes. This is based on the fact that in 0D cylinder modelling, the velocity field in the cylinder is not
evaluated based on first principles and that spatial homogeneity of the pressure is assumed as presented by Heywood [31]. In addition, with current hardware (i.e., processors in personal computers and HiL systems), the real-time capability of the engine model can be ensured with the application of single-zone [3,4] or two-zone combustion modelling [5,6,7], where the former modelling approach assumes zone-averaged properties and the latter modelling approach differentiates only between temperature and species concentrations in the burned and unburned zones [5].

General features of the proposed simplified mechanistically based spray model and innovative contributions in a 0D modelling depth can be summarized as:

1. It is based on the transient momentum equation and thus considers the influences of the injection rate.

2. It considers varying ambient parameters including the density in a quasi-steady manner.

3. It allows for modelling of spray detachment from the nozzle after the end of injection.

4. It allows for calculation of fuel mass and the mass of in-cylinder charge within selected excess air ratio limits of the spray based on first principles.

5. It allows for calculation of the fuel mass and the fraction of fuel that has reached the wall based on first principles.

It is thus worth noting that the proposed spray modelling framework models more combustion model relevant spray parameters, e.g., given in [22], relying on first principles compared to the spray models commonly used in models of similar physical depth, e.g., [6,8-12]. In addition, unlike other publications presenting spray models for system-level engine simulations, e.g., [6,8-15], this study also validates the spray model to confirm its prediction capability.

### 2.1. Governing equations

The spray model is based on the transient momentum equation that is solved analytically for the entire spray to yield a 0D spatial resolution that complies with the real-time constraint on the entire engine model as addressed previously. Derivation thus starts from the convection-driven momentum equation (assumption 6):

$$\frac{\partial}{\partial t} \int_{CV} \rho u dV = - \int_{CV} \text{div}(\rho u^2) dV,$$

(1)
where \( u \) is the spatially resolved velocity field in the spray, \( \rho \) is the density of the spray (a detailed derivation of the spray density is given in section 2.8), \( V \) is the volume and \( CV \) is the control volume defining the spray contours and thus the integration limits of the spray.

Considering assumptions 7 and 8 stating that there is only a momentum in-flux of the fuel injected from the nozzle and that the velocity profile at the nozzle is homogeneous, eq. (1) can be rearranged to

\[
\frac{\partial}{\partial t} \int_{CV} \rho u dV = \rho_{f,l} u_0^2 A_0 = \dot{M},
\]

where \( \rho_{f,l} \) is the density of the liquid fuel, \( u_0 \) is the fuel velocity at the exit of the nozzle, \( A_0 \) is the cross sectional area of the nozzle and \( \dot{M} \) is the momentum flux of the fuel through the nozzle.

In the general case, \( \dot{M} \) in eq. (2) can be a function of time, and thus the penetration \( s_{tip} \) of the circumferentially symmetrical spray – being a function of the spray momentum – is evaluated based on eq. (2) integrated over time from the beginning of injection \( (t = 0) \) until the observed time \( (t) \) as

\[
\int_{CV} \rho u dV = 2\pi \int_{s_1}^{s_{tip}} \int_0^R \rho u r dr dx = \int_0^t \dot{M} dt = \dot{M},
\]

where \( x \) represents the distance from the nozzle and \( r \) is the radial distance from the centreline of the spray \( (cl) \). Eq. (3) thus describes \( s_{tip} \) as a function of \( \dot{M} \), where \( \dot{M} \) can be an arbitrary function of time, thereby allowing for consideration of injection rate variations.

An additional two equations that provide the required inputs to the spray model describe the fuel mass as

\[
m_f = \int_{CV} c_f dV = \int_{CV} f \rho dV
\]

and the spray mass that consists of the injected fuel and entrained gas, which is in the case of an engine the in-cylinder charge:

\[
m_{sp} = \int_{CV} \rho dV,
\]

where \( c_f \) is the fuel concentration and \( f \) is the mass fraction of the fuel vapour. Eqns. (4) and (5) describe the fuel and spray mass for the entire spray as

\[
m_f = 2\pi \int_{s_1}^{s_{tip}} \int_0^R f \rho r dr dx
\]

and

\[
m_{sp} = 2\pi \int_{s_1}^{s_{tip}} \int_0^R \rho r dr dx
\]
and the fuel mass and spray mass within selected excess air ratio limits by applying relevant integration limits derived in section 2.6.2.

The analytical solution of eq. (3) in the form \( M = f_1(s_{\text{tip}}) \) can be derived for the spatially varying density \( \rho \). However, as \( f_1 \) is a relatively complex function of \( s_{\text{tip}} \), it cannot be analytically rearranged in the form \( s_{\text{tip}} = f_2(M) \), which is needed in the proposed spray modelling framework. Furthermore, in case of varying density, the solution of eq. (3) needs to be coupled with the solution of eq. (6) to obtain a solution for the system with two unknowns. As these two equations cannot be inverted explicitly, a time-consuming numerical evaluation that does not comply with real-time constraints is required to solve eq. (3) and eq. (6). Therefore, the spray with constant spatial but in general time-varying density distribution is considered further in this model; the implications of this assumption are analysed in a previous section. The time variation of density considers the time variation of the fuel vapour density (\( \rho_{f,v} \)) and the in-cylinder charge density (\( \rho_{\text{cyl}} \)) as well as the variation in spray composition, as outlined in section 2.8.

2.2. Radial distributions

Considering assumptions 1-3 and thus self-similarity of the velocity and the fuel vapour profile, the following dependencies can be derived at a certain distance from the nozzle \((x)\) [20]:

\[
\frac{u(x,r)}{u_{cl}(x)} = \frac{f(x,r)}{f_{cl}(x)} = e^{-k \left( \frac{r}{R} \right)^2}.
\]

\( R \) is determined according to assumption 5 as

\[
R = x \tan \left( \frac{\theta}{2} \right),
\]

where \( \theta \) is the spray cone angle as shown in Figure 1. In accordance with refs. [18,19], \( k \) is defined by assuming that the radial position that defines the boundary between the spray and the non-perturbed ambient corresponds to the points where the velocity is 1% of the velocity at the spray axis. The boundary between the spray and the non-perturbed ambient defines the spray radius \( R \) (Figure 1). Under the assumption that \( Sc \) is equal to unity, the same is also applicable to the fuel mass fraction. Thus,

\[
e^{-k \left( \frac{r}{R} \right)^2} = e^{-k} = 0.01
\]

yielding \( k = 4.605 \).
2.3. Axial distributions

The axial distribution of \( u_{cl}(x) \) and \( f_{cl}(x) \) is derived under the assumption of radial profiles in section 2.2 and under the assumption of constant density of the entire spray (assumption 4). For the derivation of equations in this section, first the assumption of constant boundary conditions will be made, whereas generalization of the concept is presented in section 2.4.

According to assumption 6, the momentum flux (\( \dot{M} \)) and thus the fuel mass flow (\( \dot{m}_f \)) is preserved along the centreline of the spray. The momentum flux can thus be written as

\[
\dot{M} = \int_0^R \rho u^2 dA, \tag{11}
\]

which, after inserting the velocity distribution from eq. (8) and substituting

\[
\xi = \frac{r}{r_c}, \tag{12}
\]

and

\[
y = e^{-k\xi^2}, \tag{13}
\]

yields

\[
\dot{M} = \frac{\pi \rho x^2 \tan^2 \left( \frac{\vartheta}{2} \right) u_{cl}^2(x)}{k} \int_{e^{-k}}^1 y dy = \frac{\pi \rho x^2 \tan^2 \left( \frac{\vartheta}{2} \right) u_{cl}^2(x)}{k} \left( 1 - e^{-2k} \right). \tag{14}
\]

The \( e^{-2k} \) term can be neglected as it is a small, and thus eq. (14) can be solved for \( u_{cl}(x) \), yielding

\[
u_{cl}(x) = \sqrt{\frac{2k \dot{M}}{\pi \rho \tan \left( \frac{\vartheta}{2} \right)}}. \tag{15}
\]

Following the same procedure, the fuel mass flow equation can be written as

\[
\dot{m}_f = \int_0^R \rho u f dA. \tag{16}
\]

After inserting the velocity and fuel mass fraction distribution from eq. (8) and substituting eqns. (12) and (13), eq. (16) is, following derivation procedure of eq. (14), rewritten as

\[
\dot{m}_f = \frac{\pi \rho x^2 \tan^2 \left( \frac{\vartheta}{2} \right) u_{cl}(x) f_{cl}(x)}{2k} \left( 1 - e^{-2k} \right). \tag{17}
\]

Again, \( e^{-2k} \) can be neglected. After inserting eq. (15) and rearranging, eq. (17) can be rearranged to form

\[
f_{cl}(x) = \sqrt{\frac{2k}{\pi \rho \dot{m}_f \tan \left( \frac{\vartheta}{2} \right)}}. \tag{18}
\]

2.4. Inflow boundary conditions
The momentum flux $\dot{M}$ and the density are direct inputs of the spray model (eq. (3)). As both inputs generally change during one injection, it is desired that the spray model can consider their variations. The variation of the in-cylinder temperature and pressure that affects the spray density can be substantial over the propagation period of the spray. In addition, besides rate-shaping, the momentum flux also inherently changes from the dynamics of the needle lift.

Considering eq. (3), it is obvious that the varying momentum flux can be easily considered in the lhs of the equation. Two additional parameters representing the time averaged momentum flux

$$\dot{\bar{M}} = \frac{\int_{0}^{t} \dot{M} dt}{t} = \frac{M}{t}$$

(19)

and the time averaged fuel flow

$$\dot{\bar{m}}_f = \frac{\int_{0}^{t} \dot{m}_f dt}{t} = \frac{m_f}{t}$$

(20)

are introduced to support the derivation, where $M$ and $m_f$ are given by eqns. (3) and (6), respectively. The proposed approach implies a quasi-steady propagation of the time-varying boundary conditions, as given by the convection-driven momentum equation and discussed in section 2.1.

The proposed approach allows a rearrangement of eqns. (15) and (18) to consider time-varying boundary conditions in a similar manner to eq. (3). The axial velocity and the fuel vapour distribution that ensure conservation of the fuel mass flow are thus

$$u_{cl}(x) = \sqrt{\frac{2k\dot{\bar{M}}}{\pi\rho} \frac{1}{\tan(\frac{\varphi}{2})}}$$

(21)

and

$$f_{cl}(x) = \sqrt{\frac{2k}{\pi\rho\dot{\bar{m}}_f} \frac{\dot{\bar{m}}_f}{\frac{1}{\tan(\frac{\varphi}{2})}}}$$

(22)

The conservation principle of this approach is confirmed by the fact that the injected fuel mass, i.e.,

$$m_{f,\text{inj}} = \int_{0}^{t} \dot{m}_{f,\text{inj}} dt,$$

(23)

and the fuel mass calculated by eq. (6) coincide within numerical tolerances. To ensure consistency between the injected fuel mass calculated by eq. (23) and the fuel mass calculated by eq. (6) for both (i.e., constant and time-varying) boundary conditions, the assumption of $Sc = 1$ is required.
2.5. Evaluation of $s_{\text{tip}}$

As outlined in previous sections, $s_{\text{tip}}$ is evaluated using eq. (3) and the inputs from sections 2.2-2.4. In addition to these inputs, a lower boundary of the integral in the $x$ direction (i.e., $s_1$ in eq. (3)) needs to be determined.

The applied 0D modelling depth is, similar to the 1D modelling depth, not sufficient to resolve the phenomena close to the nozzle, as the assumption on the self-similarity of the velocity and fuel vapour profile is not valid there [20]. This finding is further supported by the significant variation of the value $k$ (eq. (8)) obtained through the 3D CFD analyses near the nozzle exit ($k$ in ref. [20] represents $k/\tan\left(\frac{\theta}{2}\right)$).

In this section, $s_1$ can, for the purpose of derivation, temporarily be considered as a numerical lower boundary at which it is possible to integrate equations containing the axial velocity and the fuel vapour distribution given by eqns. (21) and (22), respectively. The modelling framework for deriving the spray dynamics and thus $s_1$ after the end of injection is presented in section 2.9, whereas the spatial positioning of $s_1$ during the injection period is elaborated in section 2.10. The parameter $s_1$ can thus be defined as the distance where $u_{cl}(s_1) = u_0$ and $f_{cl}(s_1) = 1$. Inserting either of these conditions in eqns. (21) or (22), respectively, yields

$$s_1 = \sqrt{\frac{2kM̃}{\pi\rho} \frac{1}{u_0\tan\left(\frac{\sigma}{2}\right)}}. \quad (24)$$

By applying the constant density $\rho$ and by inserting the velocity distribution from eq. (8), eq. (3) is rewritten as

$$M = 2\pi\rho \int_{s_{\text{tip}}}^{s_1} \int_{0}^{R} u_{cl}(x) e^{-k(x/R)^2} r dr dx. \quad (25)$$

After substituting eqns. (12) and (13) as well as considering the relation (21), eq. (25) is rearranged to form

$$M = \frac{\pi}{k} \rho g^2 \left(\frac{\theta}{2}\right) \sqrt{\frac{2kM}{\pi\rho} \frac{1}{\tan\left(\frac{\sigma}{2}\right)}} \int_{s_{\text{tip}}}^{s_1} x^2 \frac{1}{x} f_{cl}(s_1) dy dx \quad (26)$$

and written in the final form

$$M = \sqrt{\frac{\pi \rho M}{2k}} \tan\left(\frac{\theta}{2}\right) (1 - e^{-k}) (s_{\text{tip}}^2 - s_1^2). \quad (27)$$

The parameter $s_{\text{tip}}$ can thus be determined as
\[
S_{\text{tip}} = \sqrt{S_1^2 + \frac{M}{\sqrt{\frac{\pi \rho \dot{M}}{2k}} \tan \left( \frac{\varnothing}{2} \right) (1 - e^{-k})}},
\]

(28)

where the evaluation of \(S_1\) is described in section 2.10.

It is worth noting that for a constant injection rate, the momentum influx equation described in eq. (28) yields the relation \(S_{\text{tip}} \propto t^{0.5}\). This coincides with or is close to the data of most correlations presented in [29] and it also coincides with the long time limit presented in [28].

### 2.6. Fuel mass

#### 2.6.1 Total fuel mass

The total fuel mass is derived by applying eq. (6) and assuming constant density in the spray:

\[
m_f = 2\pi \rho \int_{S_1}^{S_{\text{tip}}} \int_0^{R} f_{cl}(x)e^{-k \left( \frac{r}{R} \right)^2} r dr dx.
\]

(29)

Following the formalism from section 2.5, eq. (29) is solved as

\[
m_f = \sqrt{\frac{\pi \rho \dot{m}_f}{2k \tilde{m}}} \tan \left( \frac{\varnothing}{2} \right) (1 - e^{-k}) \left( S_{\text{tip}}^2 - S_1^2 \right).
\]

(30)

#### 2.6.2 Fuel mass within selected excess air ratio limits

The fuel mass fraction, \(f\), can be related to the excess air ratio, \(\lambda\), via the formula

\[
f = \frac{1}{1 + \lambda L_{st}}.
\]

(31)

The radius that corresponds to a certain \(\lambda\) value at a certain distance from the nozzle \(x\) is evaluated by combining eq. (8) with eqns. (22) and (31). This yields

\[
\frac{1}{1 + \lambda L_{st}} e^{-k \left( \frac{r}{R} \right)^2} = \frac{1}{\sqrt{\frac{\pi \rho \dot{m}}{2k M} \tan \left( \frac{\varnothing}{2} \right)}},
\]

(32)

which after rearrangement gives

\[
r_{\lambda, x} = R \sqrt{\ln \left( \frac{x \tan \left( \frac{\varnothing}{2} \right)}{\frac{2k \pi \rho \dot{m} (1 + \lambda L_{st})}{\tan \left( \frac{\varnothing}{2} \right)}} \right)}.
\]

(33)

In analogy to section 2.6.1, the fuel mass in the region from the spray core up to a selected excess air ratio \(\lambda_1\) is calculated as
\[ m_{f, 0 < \lambda < \lambda_1} = 2\pi \rho \int_{s_{\lambda, min}}^{s_{\lambda, max}} \int_0^r f_c(x) e^{-k \left( \frac{r}{R} \right)^2} r dr dx, \]  

(34)

In general, it is not always possible to integrate eq. (34) between \( s_1 \) and \( s_{\text{tip}} \). Thus, the integration limits in eq. (34) should, besides the spray integration limits (i.e., \( s_1 \) and \( s_{\text{tip}} \)) also consider the excess air ratio integration limits. Therefore, \( s_{\lambda, min} \) and \( s_{\lambda, max} \) are defined as

\[
s_{\lambda, min} = \begin{cases} \bar{s}_{\lambda, min} & \text{if } \bar{s}_{\lambda, min} > s_1 \\ s_1 & \text{else} \end{cases}
\]

(35)

and

\[
s_{\lambda, max} = \begin{cases} \bar{s}_{\lambda, max} & \text{if } s_{\text{tip}} > \bar{s}_{\lambda, max} \\ s_{\text{tip}} & \text{else} \end{cases}
\]

(36)

where

\[
\bar{s}_{\lambda, min} = \sqrt{\frac{2k}{\pi \rho M}} \hat{m}_f \frac{(1 + \lambda_1 l_{st})}{\tan \left( \frac{\theta}{2} \right)} e^{-k} \]

(37)

and

\[
\bar{s}_{\lambda, max} = \sqrt{\frac{2k}{\pi \rho M}} \hat{m}_f \frac{(1 + \lambda_1 l_{st})}{\tan \left( \frac{\theta}{2} \right)}.
\]

(38)

After substituting (12) and (13), eq. (34) can be rearranged to yield

\[
m_{f, 0 < \lambda < \lambda_1} = \frac{\pi \rho tan^2 \left( \frac{\theta}{2} \right)}{k} \int_{s_{\lambda, min}}^{s_{\lambda, max}} \sqrt{\frac{2k}{\pi \rho M}} \hat{m}_f \frac{1}{\tan \left( \frac{\theta}{2} \right)} x^2 \int_1^{x \left( \frac{1 + \lambda_1 l_{st}}{2k} \right)} e^{-k \left( \frac{r}{R} \right)^2} dy dx
\]

(39)

leading to

\[
m_{f, 0 < \lambda < \lambda_1} = \frac{\pi \rho tan^2 \left( \frac{\theta}{2} \right)}{k} \sqrt{\frac{2k}{\pi \rho M}} \hat{m}_f \frac{1}{\tan \left( \frac{\theta}{2} \right)} \int_{s_{\lambda, min}}^{s_{\lambda, max}} \left( 1 - \sqrt{\frac{\pi \rho M}{2k \hat{m}_f(1 + \lambda_1 l_{st})}} \right) dx
\]

(40)

and finally to

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

(41)

The fuel mass between selected excess air ratio limits \( \lambda_1 \) and \( \lambda_2 \), where \( \lambda_2 > \lambda_1 \), is thus calculated as

\[
m_{f, \lambda_1 < \lambda < \lambda_2} = m_{f, 0 < \lambda < \lambda_2} - m_{f, 0 < \lambda < \lambda_1}
\]

(42)

2.6.3 Fuel mass reaching the walls

It is known that the fuel that has impinged on the walls can exhibit a different combustion rate [6]. To ensure that the combustion model incorporates this fact, it is necessary to determine the mass of the fuel that has reached the wall at a distance \( R_w \) from the nozzle.
Based on the common configuration of engines with central injectors it is assumed that the wall is perpendicular to the spray axis. This means that calculation of the equations in this section is performed only if the spray tip has reached the wall, i.e., if \( R_w < s_{\text{tip}} \).

In this case, \( m_{f, 0 < \lambda < \lambda_1} \), which represents the fuel mass in the region from the spray core up to a selected excess air ratio \( \lambda_1 \) that has not yet reached the wall, is calculated using eq. (41), where \( s_{\lambda_1, \text{min}} \) and \( s_{\lambda_1, \text{max}} \) are in addition to the limitations imposed in eqns. (35) and (36) limited by

\[
s_{\lambda_1, \text{min}} = \begin{cases} s_{\lambda_1, \text{min}}; & \text{if } R_w > s_{\lambda_1, \text{min}} \\ R_w; & \text{else} \end{cases}
\]

and

\[
s_{\lambda_1, \text{max}} = \begin{cases} s_{\lambda_1, \text{max}}; & \text{if } R_w > s_{\lambda_1, \text{max}} \\ R_w; & \text{else} \end{cases}
\]

where both integration limits ensure that eq. (41) is integrated only up to the wall.

The parameter \( m_{f, 0 < \lambda < \lambda_1} \) is thus calculated as specified in eq. (42) using \( m_{f, 0 < \lambda < \lambda_2} \) and \( m_{f, 0 < \lambda < \lambda_1} \), where the latter two masses are evaluated using the integration limits defined in eqns. (43) and (44). With the known values of \( m_{f, 0 < \lambda < \lambda_1} \) and \( m_{f, 0 < \lambda < \lambda_2} \) it is possible to calculate the ratio between the fuel mass that has reached the wall and the fuel mass within arbitrary excess air ratio limits – as for example specified by the excess air ratio limits \( \lambda_1 \) and \( \lambda_2 \) – by

\[
R_{f, \text{wall} \lambda_1 < \lambda < \lambda_2} = \frac{m_{f, \text{wall} \lambda_1 < \lambda < \lambda_2}}{m_{f, \lambda_1 < \lambda < \lambda_2}} = \frac{m_{f, \lambda_1 < \lambda < \lambda_2} - m_{f, 0 < \lambda < \lambda_1}}{m_{f, \lambda_1 < \lambda < \lambda_2}}.
\]

### 2.7. Spray mass

#### 2.7.1 Total spray mass

The total spray mass \( (m_{sp}) \) is derived by applying eq. (7), which is in the case of constant spray density rewritten as

\[
m_{sp} = 2\pi \rho \int_{s_1}^{s_{\text{tip}}} \int_0^R r dr dx = \pi \rho \frac{1}{3} \tan^2 \left( \frac{\theta}{2} \right) \left( s_{\text{tip}}^3 - s_1^3 \right).
\]

#### 2.7.2 Spray mass within selected excess air ratio limits

The combustion kinetics is directly influenced by the reactant concentrations. To form a basis for calculating combustion rate limiters, based on the oxygen availability within selected excess air ratio limits, it is necessary to calculate the overall mass of spray within the same excess air ratio limits \( (m_{sp, \lambda_1 < \lambda < \lambda_2}) \) that were applied in the fuel mass evaluation.
(section 2.6). The derivation is based on eq. (7), which is reformulated as outlined in section 2.7.1. The equation for \( m_{sp,0<\lambda<\lambda_1} \) thus yields

\[
m_{sp,0<\lambda<\lambda_1} = 2\pi \rho \int_0^{s_{\lambda_1,max}} \int_0^{\tau_{\lambda_1,x}} r dr dx
\]  

(47)

and

\[
m_{sp,0<\lambda<\lambda_1} = \frac{\pi \rho \tan(\frac{y}{2})}{-k A^3} \left[ \int_0^{\tau_{\lambda_1,x}} x \tan(\frac{\phi}{2}) \right] \left[ \int_0^{s_{\lambda_1,max}} \ln(\frac{1}{3}) \right] \left[ \int_0^{s_{\lambda_1,max}} \right]
\]  

(48)

After substituting

\[
y = \frac{x \tan(\frac{\phi}{2})}{\sqrt{\frac{2}{\pi \rho M} f(1+\lambda_1 L_{st})}} = Ax
\]  

(49)

the integral can be rearranged to

\[
m_{sp,0<\lambda<\lambda_1} = \frac{\pi \rho \tan^{2}(\frac{\phi}{2})}{-k A^3} \left[ \int_0^{s_{\lambda_1,max}} \ln(\frac{1}{3}) \right] s_{\lambda_1,max}^{A}
\]  

(50)

and finally to

\[
m_{sp,0<\lambda<\lambda_1} = -\frac{\pi \rho \tan^{2}(\frac{\phi}{2})}{3k} \left[ s_{\lambda_1,max} \left( \ln(s_{\lambda_1,max} A) - \frac{1}{3} \right) - s_{\lambda_1,min} \left( \ln(s_{\lambda_1,min} A) - \frac{1}{3} \right) \right].
\]  

(51)

The spray mass within selected excess air ratio limits \( \lambda_1 \) and \( \lambda_2 \), where \( \lambda_2 > \lambda_1 \), is thus again calculated as

\[
m_{sp,\lambda_1<\lambda<\lambda_2} = m_{sp,0<\lambda<\lambda_2} - m_{sp,0<\lambda<\lambda_1}.
\]  

(52)

2.8. Evaluation of spray density

As reasoned above, a constant spatial but temporally varying density distribution is assumed in the spray model. It is calculated as

\[
\rho = \frac{1}{\rho_f \frac{1}{f} - \rho_{cyl}} = \frac{\rho_{cyl}}{1 - f \left( 1 - \frac{\rho_{cyl}}{\rho_f} \right)} = \frac{\rho_{cyl}}{1 - \frac{mf}{m_{sp}} \left( 1 - \frac{\rho_{cyl}}{\rho_f} \right)}
\]  

(53)

where \( \rho_f \) is the density of the fuel vapour; \( \rho_{cyl} \) is the density of the in-cylinder charge; the fuel mass \( m_f \) and spray mass \( m_{sp} \) are given by eqns. (30) and (46), respectively; \( \rho_f \) and \( \rho_{cyl} \) are dependent on the thermodynamic properties in the cylinder; and the ratio between \( m_f \) and \( m_{sp} \) varies with spray propagation yielding the temporal density variation. The spray model is not restricted to the density evaluation according to eq. (53), and thus other relations can be applied to determine the spray density.

2.9. Spray propagation after the end of injection
In Diesel engines, combustion continues or sometimes even starts after the end of injection. The spray model therefore needs to predict fuel masses within selected excess air ratio limits after injection ends to provide a valid input to the combustion model. After the end of injection, the spray detaches from the nozzle and thus both $s_{tip}$ and $s_1$ change over time.

Turbulence phenomena cannot be represented in a 0D model. In addition, the assumption of Gaussian distribution of the velocity and the fuel concentration profile may not be valid after the end of injection. Therefore, the approach proposed below is not intended to predict fully accurately 3D contours of the spray after the end of injection but should rather be interpreted as a mechanistically motivated model that propagates the fuel from the lower to higher excess air ratios and thus makes it available for combustion. These phenomena are illustrated in section 3.3.3 and represent one of the important advantages of the proposed modelling approach compared to the system-level models cited in section 1 that do not specifically consider this phase.

Considering the 0D modelling depth and the requirement of a mechanistic modelling basis, it seems plausible to assume that the spray momentum is conserved after the end of injection, whereas the spray mass increases due to entrainment. This can be summarized in a 0D equation for propagation of the centre of gravity of the spray ($u_{cg}$) after the end of injection as

$$u_{cg} = \frac{M}{m_{sp}}.$$  \hspace{1cm} (54)

In eq. (54), $M$ remains constant and retains the value corresponding to the momentum at the end of injection, whereas $m_{sp}$ increases according to eq. (46) as the spray propagates and thus accounts for entrainment.

The derivation of the spray propagation dynamics after the end of injection is based on two steps. First, the velocity of the centre of gravity is calculated and subsequently related to the velocity of the spray tail, $\dot{s}_1$, which provides input to eq. (28) and thus enables the evaluation of $s_{tip}$ after the end of injection. The position of the centre of gravity of the spray is evaluated as

$$x_{cg} = \frac{\int_{CV} xp\,dV}{\int_{CV} p\,dV} = \frac{2\pi\rho \int_{s1}^{s_{tip}} R^2 \, \rho \, d\rho \, dx}{2\pi\rho \int_{s1}^{s_{tip}} R^2 \, \rho \, d\rho \, dx} = \frac{\pi \rho \frac{R^2}{2} (\frac{\rho}{2} (s_{tip}^4 - s_1^4))}{\frac{3}{4} (s_{tip}^4 - s_1^4)}.$$  \hspace{1cm} (55)

Differentiating eq. (55) with respect to time and introducing
\[ C = \frac{M}{\sqrt{\frac{\pi \rho M}{2k} \tan\left(\frac{\theta}{2}\right)(1-e^{-k})}} \]  

yields

\[ u_{cg} = \frac{\partial}{\partial t} x_{cg} = \frac{\partial}{\partial t} \left[ \frac{3\left(s_1^2+c^2\right)^{2-s_1^2}}{s_1^2\left(s_1^2+c^2\right)^2-s_1^2} \right] \]  

which after rearrangement gives

\[ \dot{s}_1 = \frac{4}{3} \frac{u_{cg}}{4Cs_1} \frac{s_1^2}{s_{tip}^3-s_1^3} \sqrt{\frac{2Cs_1^2+C^2}{3}} \left(s_{tip}s_1-s_1^2\right) \]  

### 2.10. Evaluation of \( s_1 \) during the injection period

In this section two approaches defining the momentum and the fuel influx from the nozzle to the spray are analysed with the aim to determine the most suitable physical position of \( s_1 \) with respect to the injector nozzle outlet. Both approaches thus relate to the boundary conditions addressed in sections 2.1 and 2.4.

Section 2.5 defines \( s_1 \) during the injection period as the distance from the nozzle where the Gaussian velocity at the centreline reaches the nozzle outlet velocity and where the Gaussian fuel vapour concentration at the centreline reaches the value of 1. In the first approach, it is assumed that there is a liquid core of length \( s_1 \) between the nozzle and the beginning of the conical spray region. In the second approach, this length will be disregarded and in analogy to the figures and ideas presented in Refs. [18,20] (a schematic comprising these ideas is presented in Figure 1), it will be assumed that the conical spray region appears immediately at the nozzle. To analyse the influence of the above assumptions, both approaches will be analysed and benchmarked against experimental results in section 3.1.

According to the basic assumption, a non-vaporizing spray is considered in the model and thus evaporation is not explicitly considered in the spray model. Therefore, no specific distinction is made between the fuel in the liquid or vapour state and thus immediately from the onset of the conical spray region a gas jet is assumed as reasoned in Ref. [18] and outlined in Section 2.1.

### 2.10.1 Considering liquid core of length \( s_1 \)

In this case, it is assumed that after the nozzle exit there is first a homogeneous liquid core of constant cross-section \( (A_0) \) and length \( s_1 \). The fuel exiting the nozzle is thus first
injected into this liquid core, which has a diameter equal to the nozzle diameter and where fuel propagates with velocity $u_{f,l}$. It is assumed that in the liquid core, the fuel is in the liquid phase and is thus incompressible. The fuel starts filling the liquid core of the length $s_1$ at the nozzle side; after the end of injection, the fuel starts emptying the liquid core again at the nozzle side. Note: the same results for the liquid core of the length $s_1$ would be obtained by assuming that the fuel is in the vapour phase and applying the equivalent diameter ($d_{eq}$) as introduced in Ref. [18]. However, this approach introduces additional complexity in the case of varying in-cylinder state as $d_{eq}$ needs to be reevaluated continuously and the continuity equation needs to be applied to consider compressibility effects.

After the liquid fuel passes the liquid core of length $s_1$, it is assumed to enter the conical spray region, whereby the momentum flux and the fuel mass flow are conserved at the boundary. The fuel is assumed to be in the vapour phase in the conical spray region. Thereby, as indicated in section 2.1, physical phenomena such as atomization, drop breakup/coalescence, drop drag and evaporation as well as their implications on the 3D flow field are neglected. Although this also influences the density distribution within the spray and spray angle, it was in section 2.1 reasoned (based on the literature) that these simplifications are acceptable within the 0-D modelling framework. Pastor et al. [20] additionally indicated that the sprays in modern Diesel engines, which are characterised by high boost and injection pressure as well as small nozzle hole diameter, can be analysed from the point of view of the gas jet theory even under non-vaporising conditions. The presented ideas can be summarized in the following framework of governing equations for the incompressible liquid core of length $s_1$. The momentum equation is derived from eq. (1) or analogously eq. (2) as

$$\dot{M} = \dot{M}_{nozzle} - \frac{\partial}{\partial t} \int_{CV} \rho udV = \dot{M}_{nozzle} - \rho_{f,l} A_0 \frac{\partial (u_{f,l} x_{f,l})}{\partial t},$$

(59)

where $\dot{M}_{nozzle}$ is the momentum flux at the exit nozzle and $\dot{M}$ is the momentum flux at the interface between the liquid core and the conical spray region, which is used as the boundary condition in eq. (3). The difference between these two momentum fluxes is in the last term of eq. (59), which accounts for momentum variation in the incompressible liquid core of the length $s_1$. In the liquid core fuel propagates with velocity $u_{f,l}$, and $x_{f,l}$ denotes the length of the actual fuel core within the liquid core of length $s_1$.

To properly address the dynamic phenomena within the liquid core, it is necessary to derive a framework for evaluating $x_{f,l}$. It is thus necessary to account for fuel propagation within the liquid core of length $s_1$, i.e., for filling the liquid core during the initial injection
period, indicated by the increase of $x_{f,l}$ from 0 to $s_1$, and likewise for emptying the liquid core after the end of injection, indicated by the decrease of $x_{f,l}$ from $s_1$ to 0.

During the injection period, $x_{f,l}$ is therefore defined as

$$ x_{f,l} = \begin{cases} s_1 \frac{m_{f,\text{inj}}}{m_{f,l}}; & \text{if } m_{f,l} > m_{f,\text{inj}} \\ s_1; & \text{else} \end{cases} $$

(60)

where $m_{f,\text{inj}}$ is given by eq. (23) and $m_{f,l}$ is the fuel mass within the liquid core of length $s_1$ and is defined as

$$ m_{f,l} = \rho_{f,l} A_0 s_1. $$

(61)

It should be noted that $s_1$ can vary because of variations in $\dot{M}$, $\rho$ or $u_0$ that influence $s_1$ via eq. (24).

After the end of injection, a liquid fuel that propagates towards the conical spray region is still present within the liquid core of length $s_1$. In this case, $x_{f,l}$ is calculated as

$$ x_{f,l} = s_1 \left( 1 - \frac{m_{f,l,\text{out},\text{EOI}}}{m_{f,l}} \right), $$

(62)

where the mass of liquid fuel that has left the liquid core after the end of injection ($m_{f,l,\text{out},\text{EOI}}$) is calculated as

$$ m_{f,l,\text{out},\text{EOI}} = \int_{t_{\text{EOI}}}^{t_{\text{EOI}}+t^*} \rho_{f,l} A_0 u_0 dt $$

(63)

where $t_{\text{EOI}}$ is the time at the end of injection, $t^*$ is the time after the end of injection and $u_0$ has a constant value (as stated in eq. (63)) equal to the injection velocity at the last time step of the injection event. Eq. (63) is integrated until $m_{f,l,\text{out},\text{EOI}} = m_{f,l}$, indicating that there is no fuel left in the liquid core.

2.10.2 No liquid core

As indicated in section 2.10, in this second case it is assumed that $s_1$ is translated to the nozzle exit, as shown in Figure 1. Thereby it is assumed that the spray features a conical shape already at the nozzle exit. Therefore, the coordinate system of the spray does not originate at the nozzle exit but at the distance $-s_1$ from the nozzle exit (Figure 1). This approach can be justified by the fact that high injection pressures promote a complete atomization regime inside the spray near the nozzle exit [20] and thus the liquid core of length $s_1$ need not be considered. This approach is compatible with the modelling approach proposed in [20]. Inflow boundary conditions of the spray model (sections 2.1 and 2.4) are in
this case determined solely by the injection rate and directly yield $\dot{M}$ and $u_0$, as shown in Figure 1.

3. Results and Discussion

In this section, validation results for the spray model are presented first. Subsequently, features of the spray model are demonstrated.

3.1. Impact of the evaluation procedure of $s_1$ on the $s_{tip}$

The impact of the evaluation procedure of $s_1$ is presented first, as it decisively influences the results of the spray model. The results in Figure 2 clearly demonstrate that much better agreement with the experimental data on the spray tip penetration is obtained if the approach proposed in section 2.10.2 (i.e., assuming the conical spray shape already at the nozzle exit) is applied instead of the approach proposed in section 2.10.1. This indicates that the approach that assumes the conical spray appears immediately at the nozzle as indicated in [18,20] is more suitable within the proposed modelling framework and when modelling sprays encountered in modern engines. Therefore, in the subsequent sections only the results related to the approach proposed in section 2.10.2 will be discussed.

3.2. Model validation

In addition to the initial validation case presented in section 3.1, more comparisons of measured and simulated data are presented in this section to confirm the capability of the model to plausibly predict spray tip penetration for various injection and ambient parameters. In this section, the term “ambient” will be used and not the “in-cylinder charge” as experimental data used for validation were not measured in the cylinder of an engine. Again, spray tip penetration data are used for model validation.

Experimental data from two different data sources, i.e., [18,28] where exact data from [28] were downloaded from [32], were used to reduce the potential impact of source-specific biases. However, it should be noted that experimental data were not measured by the author and lack information on the measurement uncertainties. Data sets were selected in a way that each of the data sets was measured at a different but approximately constant injection pressure and varying ambient density. Experimental data of non-vaporizing and non-reacting sprays were used for model validation to comply with the physical depth of the modelling
framework. For comparisons to the experimental results (Figures 2-7), the injection pressure, the ambient density and the spray cone angle were used as inputs to the simulation model, whereas pressure and temperature were additionally used to calculate the fuel vapour density in eq. (53). In cases analysed in Figures 2-7, the fuel is injected over the entire observed period.

It is discernible from Figures 2-7 that modelled results agree well with the measured data of both data sets. Although there is in general good agreement between modelled and measured data, regions where both curves feature a different gradient, i.e., the spray tip propagation velocity, can also be observed in certain figures. These differences can to a certain extent be related to the assumptions listed in section 2, and it can in general be concluded that the modelled and measured results coincide well considering the limitations of the 0D modelling approach and the real-time capability of the spray model.

It is important to note that the model is capable of correctly predicting a decrease in spray tip penetration for an increasing ambient density for both injection pressures. In addition, the figures indicate that the proposed model adequately predicts spray dynamics on the level of accuracy adopted for system-level application. This conclusion is valid despite the fact that the proposed framework does not consider the short time scale propagation regime $s_{tip} \propto t$ [28]. Because of the high ambient densities and resulting short time scale, this propagation regime does not have a significant impact on spray penetration at the temporal and spatial scales relevant for combustion modelling in high speed Diesel engines. It can thus be concluded that the proposed model is capable of predicting the spray tip penetration of non-vaporizing sprays with high accuracy at the temporal and spatial scales relevant for combustion modelling in high speed Diesel engines.

In Figures 2-7, the time scale of 1 ms was selected to ensure sufficient readability at shorter time scales, which are of interest because of the different propagation regimes presented in [28] and discussed in section 2.5. However, Figures A1 and A2 (presented in Appendix A) additionally confirm that the model is capable of adequately predicting the spray tip penetration of non-vaporizing sprays at spatial scales larger than the mean free spray path in automotive engines.

3.3. Features of the spray model

This section demonstrates features of the spray model and innovative contributions provided by the 0D model as listed in the Introduction. The results in this section should be
assessed while considering the model assumptions outlined in sections 2 and 2.9 and the scope of the model, which is to predict masses of fuel within selected limits of excess air ratios during and after the end of injection.

3.3.1 Influence of the injection rate on spray propagation

This section presents the influence of three different injection rates, i.e., constant, increasing and decreasing, on spray tip penetration. Analysed injection rates are shown in Figure 8, whereas Figure 9 shows corresponding spray tip penetrations. Injection rates were selected in a way to ensure an approximately constant injected amount of fuel over the injection period of 1 ms. By analysing both figures, it can be concluded that for high injection rates in the initial injection phase, the spray tip propagates faster in that phase and vice versa. Considering equations derived in section 2.6 and in particular in section 2.6.2, it can thus be concluded that higher injection rates in the initial injection phase result in more fuel being mixed to higher excess air ratios and thus more fuel being available for combustion. This would lead to a more intense ROHR in the early combustion phase, whereas the inverse trend is characteristic for higher injection rates towards the end-of-injection (EOI). These plausible responses of the spray model on the injection rate-shaping are a prerequisite for assessing the influence of injection rate-shaping using a system-level engine model. It is worth noting that plausible responses of the spray model can be achieved despite neglecting the delays in information propagation as outlined in sections 2 and 2.4.

3.3.2 Spray propagation

In this section the results of the spray propagation during the injection period and after the end of injection are presented for a realistic injection profile of a modern engine. The results are shown for a nozzle with a diameter of 0.159 mm and an injection pressure of 1200 bar. Figure 10 indicates that until EOI the spray tip ($s_{tip}$) advances faster than after the EOI, which is in agreement with the governing equations proposed in sections 2.5 and 2.9. In agreement with the approach proposed in section 2.10.2, $s_{1}$ is zero during the injection period. After EOI the spray detaches from the nozzle and propagates as proposed in the modelling approach of section 2.9. Moreover, it can also be observed that first $s_{tip}$ and afterwards also $s_{1}$ reach the wall (which in this illustrative example is set at a distance $R_w = 0.04$ m) indicating that the entire spray has reached the wall.
3.3.3 Fuel masses within selected excess air ratio limits

This section comprises results related to the fuel masses within selected excess air ratio limits, which are required to provide inputs to the advanced MCC model. In this example, results for \( \lambda_{\text{low}} = 0.25 \), \( \lambda_{\text{hi}} = 1 \) and \( \lambda_{\text{R}} \), which corresponds to the outer spray boundary defined by eq. (9), are shown, whereas the spray model is applicable to an arbitrary number of excess air ratio limits. Figure 11 indicates that \( m_{f,0<\lambda<\lambda_{\text{low}}} \) increases immediately after SOI, whereas \( m_{f,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} \) and \( m_{f,\lambda_{\text{hi}}<\lambda<\lambda_{\text{R}}} \) increase with some delay as the spray tip advances (Figure 10), which coincides with the spray dynamics analysed in section 3.3.2. Moreover, it can be observed that after EOI (\( s_1 > 0 \) in Figure 10) \( m_{f,0<\lambda<\lambda_{\text{low}}} \) drops to zero as a consequence of the spray dynamics and thus because of air or in-cylinder charge entrainment into the spray. Similarly, \( m_{f,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} \) decreases as well and thus with prolonged time after EOI all the fuel is gradually mixed with air or in-cylinder charge above \( \lambda_{\text{hi}} \).

3.3.4 Fuel masses within selected excess air ratio limits – wall interaction

In addition to the results shown in Figure 11, Figure 12 and also Appendix B show masses of the fuel that has reached the wall (at a distance \( R_w = 0.04 \) m as presented in Figure 10). Figure 12 clearly indicates that \( m_{f,\text{wall},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} \) and \( m_{f,\text{wall},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} \) start increasing when the spray reaches the wall (\( s_{\text{tip}} > R_w \) in Figure 10), whereas after the entire spray has reached the wall (\( s_1 > R_w \) in Figure 10) \( m_{f,\text{wall},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} = m_{f,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} \) and \( m_{f,\text{wall},\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} = m_{f,\lambda_{\text{low}}<\lambda<\lambda_{\text{hi}}} \), clearly indicating that all the fuel has reached the wall. In the analysed case fuel is mixed to a higher excess air ratio than 0.25 before it reaches the wall. Therefore, \( m_{f,\text{wall},\lambda<\lambda_{\text{low}}} \) is always zero and thus is not shown in Figure 12.

4. Conclusions

In this paper, a mechanistically based spray model capable of predicting the mass of fuel within arbitrarily selected limits of excess air ratios during and after the end of injection is presented. The model is based on a 0D non-vaporizing and non-reacting modelling framework. The main characteristics of the spray model can be summarized as:

1. The spray model is based on the transient momentum equation. It is therefore capable of considering the influences of injection rate shaping on the spray parameters and
consequently on the mass of fuel within selected limits of excess air ratios. Thereby it is possible to simulate the influence of the injection rate on the burn rate.

2. The spray model allows for consideration of varying ambient parameters in a quasi-steady manner.

3. A modelling framework for simulating the spray detachment from the nozzle after the end of injection is proposed in the paper. This model is crucial for a plausible prediction of the fuel mass and the mass of in-cylinder charge within selected excess air ratio limits after the end of injection, when progressively more air or in-cylinder charge entrains the spray.

4. An analytical framework for determining the fuel mass that has reached the wall is derived. It enables calculation of the amount of fuel that can be subjected to a wall specific treatment in the combustion model.

The spray model was successfully validated against measured data of non-vaporizing spray for varying injection parameters and ambient densities, thus confirming its predictive capability. It can be concluded that the presented spray model is a plausible and generally applicable input module for computationally fast mixture-controlled-combustion models on the system level.

Acknowledgment

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References


Appendix A

Figures A1 and A2 confirm the capability of the spray model to adequately predict the spray tip penetration of non-vaporizing sprays for longer times over which spray tip penetration exceeds the mean free spray path in the automotive engines.

Appendix B

Appendix B summarizes numerical data of the curves shown in Figure 12 to present numerical data more clearly.

Table 1 Fuel masses presented in Figure 12 as a function of time

<table>
<thead>
<tr>
<th>time [ms]</th>
<th>( m_f ) [mg]</th>
<th>( m_{f,0&lt;\lambda&lt;\lambda_{low}} ) [mg]</th>
<th>( m_{f,\lambda_{low}&lt;\lambda&lt;\lambda_{hi}} ) [mg]</th>
<th>( m_{f,\lambda_{hi}&lt;\lambda&lt;\lambda_{low}} ) [mg]</th>
<th>( m_{f,wall,\lambda_{low}&lt;\lambda&lt;\lambda_{hi}} ) [mg]</th>
<th>( m_{f,wall,\lambda_{hi}&lt;\lambda&lt;\lambda_{low}} ) [mg]</th>
<th>( m_{f,wall,\lambda_{low}&lt;\lambda&lt;\lambda_{hi}} ) + ( m_{f,wall,\lambda_{hi}&lt;\lambda&lt;\lambda_{low}} ) [mg]</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.0</td>
<td>0.00</td>
<td>0.00</td>
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<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.2</td>
<td>0.4</td>
<td>0.20</td>
<td>0.21</td>
<td>0.08</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.4</td>
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<td>0.27</td>
<td>0.88</td>
<td>0.41</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.6</td>
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<td>0.29</td>
<td>1.54</td>
<td>0.91</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>0.8</td>
<td>3.9</td>
<td>0.30</td>
<td>2.11</td>
<td>1.56</td>
<td>0.00</td>
<td>0.00</td>
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</tr>
<tr>
<td>1.0</td>
<td>5.1</td>
<td>0.31</td>
<td>2.55</td>
<td>2.26</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>1.2</td>
<td>6.4</td>
<td>0.31</td>
<td>2.96</td>
<td>3.15</td>
<td>0.22</td>
<td>0.55</td>
<td>0.77</td>
</tr>
</tbody>
</table>
Figure 1 Schematic of the spray geometry with nozzle exit at $x = s_1$, which corresponds also to the spray origin as discussed in section 2.10.2.
Figure 2 Comparison of the simulated results with (section 2.10.1) and without (section 2.10.2) consideration of the liquid core and measured results (Ref. [18]) for an injection pressure of 800 bar, an ambient density of 24 kg/m³ and a spray cone angle of 22 deg.
Figure 3 Comparison of the simulated and measured results for an injection pressure of 800 bar, an ambient density of 46 kg/m³ and a spray cone angle of 23 deg (measured results from Ref. [18])
Figure 4 Comparison of the simulated and measured results for an injection pressure of 800 bar, an ambient density of 69 kg/m³ and a spray cone angle of 25 deg (measured results from Ref. [18])
Figure 5 Comparison of the simulated and measured results for an injection pressure of 1420 bar, an ambient density of 51.9 kg/m³ and a spray cone angle of 25.59 deg (measured results from Ref. [28])
Figure 6 Comparison of the simulated and measured results for injection pressure of 1440 bar, an ambient density of 75.3 kg/m$^3$ and a spray cone angle of 29.58 deg (measured results from Ref. [28])
Figure 7 Comparison of the simulated and measured results for an injection pressure of 1410 bar, an ambient density of 122 kg/m³ and a spray cone angle of 28.93 deg (measured results from Ref. [28])
Figure 8 Injection rates of constant, increasing and decreasing injection profiles
Figure 9 Spray tip penetration for injection rates presented in Figure 8
Figure 10 Time evolution of $s_1$ and $s_{tip}$ with indicated wall ($R_w = 0.04 \text{ m}$)
Figure 11 Time evolution of the injected fuel ($m_f$) and masses of fuel within selected excess air ratio limits
Figure 12 Time evolution of the injected fuel ($m_f$), masses of fuel within selected excess air ratio limits and mass of fuel that has reached the wall.
Figure A1 Comparison of the simulated and measured results for injection pressure of 1440 bar, an ambient density of 75.3 kg/m³ and a spray cone angle of 29.58 deg (measured results from Ref. [28])
Figure A2 Comparison of the simulated and measured results for injection pressure of 1410 bar, an ambient density of 145 kg/m³ and a spray cone angle of 32.13 deg (measured results from Ref. [28])