A Reduced-order Model for Multiphase Simulation of Transient Inert Sprays

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Abstract

In global efforts to reduce harmful greenhouse gas emissions from the transportation sector, novel bio-hybrid liquid fuels from renewable energy and carbon sources can be a major form of energy for future propulsion systems due to their high energy density. A fundamental understanding of the spray and mixing performance of the new fuel candidates in combustion systems is necessary to design and develop the fuels for advanced combustion concepts. In the fuel design process, a large number of candidates is required to be screened to arrive at potential fuels for further detailed investigations. For such a screening process, three-dimensional (3D) simulation models are computationally too expensive and hence unfeasible. Therefore, in this paper, we present a fast, reduced-order model for inert sprays. The model is based on the cross-sectionally averaged spray (CAS) model derived by Wan (1997) from 3D multiphase equations. The original model was first tested against a wide range of conditions and different fuels. The discrepancies between the CAS model and experimental data are addressed by integrating state-of-the-art breakup and evaporation models. In addition, a transport equation for vapor mass fraction is proposed, which is important for evaporation modeling. Furthermore, the model is extended to consider polydispersed droplets by modeling the droplet size distribution by commonly used presumed probability density functions, such as Rosin-Rammler, lognormal, and gamma distributions. The improved CAS model is capable of predicting trends in the macroscopic spray characteristics for a wide range of conditions and fuels. The computational cost of the CAS model is lower than the 3D simulation methods by up to 6 orders of magnitude depending on the method. This enables the model to be used not only for the rapid screening of novel fuel candidates, but also for other applications, where reduced-order modeling is useful.

Keywords: Reduced-order model, CAS, inert spray, droplet size distribution, bio-hybrid fuels

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1. Introduction

With increasing concerns about the environment due to rising global temperatures, greenhouse gas (GHG) emissions from the transportation sector are among the targets of stringent control as recommended by international governing institutions (EU Commission, 2018). According to the Intergovernmental Panel on Climate Change (IPCC) (2014) report, the transportation sector contributes approximately 23% of total global GHG emissions. This share is going to become larger with increasing demand unless mitigation efforts are made to develop low-carbon fuels and energy-efficient propulsion systems. Burning fossil fuels, such as gasoline and diesel, contributes a vast amount to this energy demand (U. S. Energy Information Administration, 2016).

To reduce direct GHG emissions from internal combustion engines (ICEs), powertrain electrification is emerging as an alternative. However, the life-cycle assessment studies of electric vehicles show that such vehicles are still not economically viable and cannot reduce overall well-to-wheel emissions if the electricity is generated mainly from fossil sources (Rupp et al., 2018, 2019, 2020; Helmers et al., 2020). Therefore, a mix of propulsion technologies is required to meet the well-to-wheel emissions reduction (Senecal and Leach, 2019). This implies that ICEs will remain important primary sources of power in conventional as well as hybrid propulsion systems. To reduce their environmental impact, it is necessary to develop carbon-neutral fuels and improve combustion engines through new combustion concepts that enhance efficiency and reduce pollutant emissions.

Global research programs, such as Co-Optimization of Fuels and Engines (Co-Optima, 2020) and Future Energy Systems (2020) among others, are developing low-carbon fuels and highly efficient engine concepts. Similarly, the Cluster of Excellence, “The Fuel Science Center” (FSC, 2020) at RWTH Aachen University, aims to integrate renewable electricity with a combined utilization of carbon dioxide (CO₂) and carbon sources from ligno-cellulosic biomass to produce new high-density liquid energy carriers dubbed as bio-hybrid fuels. Together with the new bio-hybrid fuels, innovative engine concepts are being developed for highly efficient and clean combustion processes.

In the fuel design process, fuels need to be tested for their applicability in conventional as well as new combustion concepts. Such testing and validation of all potential fuel candidates is not always possible at the engine test bench due to several reasons. The new fuel candidates may not be available in large quantities initially, and only molecular structure is known from proposed production processes. Also, combustion systems may need to be adapted before extensive testing. Since the atomization of the liquid fuel jet and its subsequent mixture formation is an essential intermediate step towards combustion and emissions, simplified experiments for spray breakup and mixing can be performed under engine-like conditions in a constant volume or constant pressure chamber to reduce the required amount of fuel. However, even such experiments can be impractical for a large number of
candidates for the same reasons as mentioned before. In this case, predictive numerical simulations of spray and mixture formation can be useful for assessing the performance of fuel candidates in engine-like conditions. Such simulations, depending on the method and approach, may be computationally expensive, e.g., direct numerical simulation (DNS) of an ICE with a full injection system is intractable with current state-of-the-art computing resources available worldwide. These simulations may be feasible with large-eddy simulation (LES) or Reynolds-averaged Navier-Stokes (RANS) approach. Still, it may not be practical to perform such simulations for each fuel candidate. Reduced-order models can provide trends and initial estimates to evaluate a large number of potential novel fuel candidates. A small number of fuel candidates can be selected with the initial screening for further more detailed investigations.

The development of control strategies is an integral part of the combustion system development. Adaptive control strategies can potentially help to run combustion devices with optimal efficiency in real time to meet performance and emission targets. Adapting to the strongly non-linear nature of the chemical and physical processes in combustion requires sophisticated model-based closed-loop control strategies, e.g., in the context of diesel and dual-fuel engines (Albrecht et al., 2007; Bengtsson et al., 2007; Hillion et al., 2009; Ritter et al., 2017; Korkmaz et al., 2018a,b). In this case, reduced-order models, acting as a digital twin of the combustion system, can provide physics-based predictions to the controller to adjust the input parameters.

Thus, simplified yet reliable physics-based models find application in many areas including but not limited to the rapid screening of novel bio-hybrid fuel candidates and physics-based closed-loop control of the energy conversion devices.

1.1. State-of-the-art

The pathway from delivery of the fuel into the combustion engine through to the emission of exhaust gases out of the engine can be divided into several stages: fuel jet primary breakup and atomization; evaporation; mixing of fuel with the ambient gas; ignition; combustion; and pollutant formation. In this paper, we focus on jet primary breakup and atomization, evaporation, and mixing processes. The fuel spray can be characterized in terms of different global parameters, such as liquid and vapor penetration length, droplet size distribution, distribution of fuel vapor mass fractions along the spray axis. These quantities depend on thermo-physical properties of the fuel and directly influence further mixing, combustion, and pollutant formation. Several early studies on diesel sprays investigated macroscopic characteristics of sprays experimentally (Wakuri et al., 1959, 1960; Hiroyasu and Arai, 1980) and developed correlations for the spray tip penetration, spray angle, breakup time, and droplet size distribution. Further modeling efforts (Dent, 1971; Hay and Jones, 1972; Naber and Siebers, 1996) developed power laws for the spray tip penetration with respect to time, nozzle exit
diameter, the pressure difference across the nozzle, density of fuel, and ambient density. Sazhin et al. (2001) derived approximate analytical expressions for the spray tip penetration in initial stages as well as fully developed flow. The authors modeled the initial stage as the single phase flow dominated by the liquid phase and later stages as the two-phase flow. It was found that the diesel spray could be described solely on the basis of a two-phase approximation throughout all stages, as the fuel jet breaks up immediately after leaving the nozzle. Later, simplified models were developed for the macroscopic characterization of diesel sprays (Desantes et al., 2006). Pastor et al. (2008) developed a one-dimensional Eulerian model for transient inert sprays based on the assumption of locally homogeneous and mixing-controlled processes. Desantes et al. (2009) extended this model to reactive diesel sprays and later to multicomponent fuels (Pastor et al., 2015). Musculus and Kattke (2009) extended the steady-state control volume approach of Naber and Siebers (1996) to transient non-vaporizing sprays to study entrainment waves at the end of injection. Xu et al. (2016) extended the steady-state homogeneous control volume approach to consider the heterogeneous distribution of velocity and fuel volume fraction over the cross-section, which improved the prediction of liquid length.

1.2. Scope and Objectives

Most of the previous studies focused on modeling of diesel jets using simplified approaches derived from conservation of mass, momentum, and energy fluxes across the control volumes along the axis of the spray. With the exception of Sazhin et al. (2001), other models neglected droplet dynamics assuming homogeneous two-phase mixture. These models were originally derived for one-dimensional (1D) systems. Wan (1997) followed a top-down approach for model reduction and derived a 1D cross-sectionally averaged spray (CAS) model for two-phase diesel spray from the three-dimensional (3D) multiphase model. The model considered most of the important processes, such as droplet drag, breakup, evaporation, and entrainment, and was applied to both non-vaporizing and vaporizing sprays for prediction of macroscopic spray characteristics (Wan and Peters, 1997, 1999). In addition, it was also interactively coupled with a 3D computational fluid dynamics (CFD) code to model the near-nozzle dense spray region (Hasse and Peters, 2002; Hasse et al., 2003). The reduced-order modeling with a description of all physical processes relevant to transient inert sprays makes it particularly suited for the application to a wide range of fuels and conditions, including those where near-nozzle dense spray modeling is important and droplet dynamics cannot be neglected.

Along these lines, the objectives of this paper are twofold: (1) to evaluate the original CAS model for modern injection systems and novel fuel candidates; and (2) to propose crucial improvements to the model to increase its applicability to a wide range of conditions and fuels. This paper focuses on inert sprays as the first part of a series of two papers on the reduced-order spray model for inert and turbulent reactive sprays.
The remaining article is arranged as follows. In Section 2, the new improved CAS model is presented. Section 3 describes the measurement cases, experimental methods, and 3D simulation methods and data used for validation. The results of the original and the newly developed CAS model are discussed in Section 4. Finally, the paper finishes with a summary and conclusions. For completeness and further reference, the original CAS model and some results are included in Appendix A.

2. Models and Methods

Inspired by the analysis of jet flames, Wan (1997) proposed a radially integrated multiphase formulation for non-vaporizing and vaporizing sprays, termed as CAS model, which has been shown to work well for diesel-like engine conditions (Wan and Peters, 1997, 1999; Hasse and Peters, 2002; Hasse et al., 2003). Under the boundary layer assumptions, the density-weighted cross-sectional average of the quantity of interest, \( \phi \), is defined as

\[
\bar{\rho} \hat{\phi} b^2 = 2 \int_0^\infty \rho \phi r dr ,
\]

where \( \rho \) is the density, \( b(z, t) \) the spray half-width, \( r \) the radial coordinate, \( z \) the axial coordinate, and \( t \) the temporal coordinate. The ‘overline’ operator \( \bar{} \) and the ‘hat’ operator \( \hat{} \) denote cross-sectional averaging (with \( \phi = 1 \)) and density-weighted cross-sectional averaging, respectively, as defined in Eq. (1). The radially integrated multiphase differential operator is defined for each phase as

\[
D_{\text{phase}} (\bar{\rho} \hat{\phi} b^2) = \frac{\partial}{\partial t} (\bar{\rho} \hat{\phi} b^2) + \frac{\partial}{\partial z} (\bar{\rho} \hat{\phi} u_{\text{phase}} b^2) \quad \text{with phase} = g, l,
\]

where subscripts ‘g’ and ‘l’ denote gaseous and liquid phase, respectively. All quantities are assumed to be uncorrelated in the radial direction, which simplifies the evaluation of radial integrals of joint quantities.

2.1. Governing Equations

In the original work of Wan (1997), multi-dimensional equations for a complete spray (Hiroyasu and Arai, 1980) were radially integrated, assuming boundary layer approximations, azimuthal symmetry, and top-hat profiles for all flow variables. A detailed description of the original CAS model including the models for droplet breakup and evaporation and the comparison of its performance with respect to LES and URANS simulations is reported in Appendix A. The original governing equations for the CAS model (Eq. (A.1)-(A.6)) did not explicitly compute the vaporized fuel mass fraction, which can have a significant impact on the evaporation process through the change in gas mixture properties. The spray modeling has progressed significantly since the CAS model was first proposed in 1997, especially in the spray breakup and evaporation modeling. In this work, several advances are proposed to improve
the model predictions for the current fuel injection systems. Current state-of-the-art models for spray breakup and evaporation models were integrated into the CAS model. An additional equation is solved for the fuel-vapor transport, which is essential for the accurate modeling of evaporation rates. Here, a new approach is developed to consider different droplet sizes instead of just assuming that the spray is monodisperse. The new improved CAS model is described by the following system of hyperbolic partial differential equations (PDEs) with source terms:

\[ D_l(\bar{\rho} \hat{Y}_l b^2) = \dot{\omega}_{\text{ent},a} b \]  
(3)  
\[ D_g(\bar{\rho} \hat{Y}_g b^2) = \langle \dot{\omega}_{\text{vap}} \rangle b^2 \]  
(4)  
\[ D_g(\bar{\rho} \hat{Y}_a \hat{u}_g b^2) = -\langle \dot{\omega}_{\text{drag}} \rangle b^2 + \langle \dot{\omega}_{\text{vap}} \rangle \hat{u}_l b^2 \]  
(5)  
\[ D_l(\bar{\rho} \hat{Y}_l b^2) = -\langle \dot{\omega}_{\text{vap}} \rangle b^2 \]  
(6)  
\[ D_l(\bar{\rho} \hat{Y}_l \langle \hat{u} \rangle b^2) = \langle \dot{\omega}_{\text{heat}} \rangle b^2 - \langle \dot{\omega}_{\text{vap}} \rangle \hat{u}_l b^2 \]  
(7)  
\[ D_l(\bar{\rho} \hat{Y}_l \langle \hat{d} \rangle b^2) = -\langle \dot{\omega}_{\text{bre}} \rangle b^2 - \frac{4}{3} \langle \dot{\omega}_{\text{vap}} \hat{d} \rangle b^2 \]  
(8)  
\[ D_l(\bar{\rho} \hat{Y}_l \langle \hat{T}_d \rangle b^2) = \langle \dot{\omega}_{\text{heat}} \rangle b^2 - \langle \dot{\omega}_{\text{vap}} \hat{T}_d \rangle b^2 \]  
(9)  
\[ D_l(\bar{\rho} \hat{Y}_l \langle \hat{d} \rangle b^2) = -\langle \dot{\omega}_{\text{bre}} \rangle b^2 - \frac{4}{3} \langle \dot{\omega}_{\text{vap}} \hat{d} \rangle b^2 \]  
(10)  

The quantity \( \phi \) has been replaced by individual or combinations of the flow variables, such as the mass fractions \((Y_{a,v,l})\) and the velocities \((u_{g,l})\) of the respective phases, the droplet diameter \((\hat{d})\), and the droplet temperature \((\hat{T}_d)\) to obtain the set of PDEs. The subscript ‘d’ marks the droplet variables. Any term, \( \zeta(\hat{d}) \), which depends on the droplet diameter, is integrated over the droplet size distribution, \( \mathcal{P}(\hat{d}) \), as

\[ \langle \zeta \rangle = \int \zeta(\hat{d}^\prime) \mathcal{P}(\hat{d}) d\hat{d}^\prime, \]  
(11)  

where the operator, \( \langle \cdot \rangle \), defines the expectation value of \( \zeta(\hat{d}) \). The subscripts ‘a’ and ‘v’ denote ambient gas and vapor, respectively. Mass conservation requires \( \hat{Y}_l + \hat{Y}_v + \hat{Y}_a = 1 \) and \( \hat{Y}_g = \hat{Y}_v + \hat{Y}_a \). The two-phase cross-sectionally averaged mixture density is computed as

\[ \frac{1}{\bar{\rho}} = \frac{\hat{Y}_l}{\rho_l} + \frac{\hat{Y}_v}{\rho_v} + \frac{\hat{Y}_a}{\rho_a}, \]  
(12)  

where \( \rho_{l,v,a} \) denote densities of liquid, vapor, and ambient gas, respectively. The spray half-width, \( b(z,t) \), is computed by local mass conservation by summation of Eq. (3), Eq. (4), and Eq. (6) and then using the mixture density \( \bar{\rho} \). The source terms on the right-hand side, represent different models for physical processes, namely, entrainment \( (\dot{\omega}_{\text{ent},a}) \), drag \( (\dot{\omega}_{\text{drag}}) \), evaporation \( (\dot{\omega}_{\text{vap}}) \), droplet breakup \( (\dot{\omega}_{\text{bre}}) \), and droplet heating \( (\dot{\omega}_{\text{heat}}) \). The physical sub-models used are described briefly in the next subsections.
2.2. Entrainment Model

Entrainment of the ambient gas into the spray plume leads to its spreading in the radial direction, which develops the spray cone angle. The source term for entrainment is modeled as \( \dot{\omega}_{\text{ent,a}} = \rho_a \beta \hat{u}_g \) with spreading coefficient, \( \beta = \tan(\theta/2) \), depending on the spray cone angle, \( \theta \). Several correlations for the spray cone angle were discussed by Wan (1997), eventually using values interpolated from Naber and Siebers (1996). In this study, the correlation by Hiroyasu and Arai (1980) is used, which considers the effects of nozzle internal geometry on the spray cone angle, neglecting cavitation effects and has been shown to closely match with the experimental data. The spray cone angle (\( \theta \), in degree) is given as

\[
\theta = C_{\text{noz}} \left( \frac{\rho_a}{\rho_l} \right)^{0.26},
\]

where

\[
C_{\text{noz}} = 83.5 \left( \frac{L_{\text{noz}}}{D_{\text{noz}}} \right)^{-0.22} \left( \frac{D_{\text{noz}}}{D_{\text{sac}}} \right)^{0.15},
\]

with \( L_{\text{noz}} \) as the length of the nozzle orifice, \( D_{\text{noz}} \) as the nozzle exit diameter, and \( D_{\text{sac}} \) as the nozzle sac diameter.

2.3. Drag Model

The total steady-state drag force on a droplet of diameter \( d \) is computed as (Wan, 1997; Crowe et al., 2012)

\[
\dot{\omega}_{\text{drag}} = 3C_{\text{drag}} \rho_g \hat{Y}_l (\hat{u}_g - \hat{u}_l) |\hat{u}_g - \hat{u}_l| 4\rho d.
\]

The droplet drag coefficient, \( C_{\text{drag}} \), depends on the droplet Reynolds number, \( \text{Re}_d \), as (Wallis, 1969)

\[
C_{\text{drag}} = \begin{cases} 
24 \left( \frac{1}{\text{Re}_d} \right) (1 + \frac{1}{6} \text{Re}_d^{2/3}) & \text{for } \text{Re}_d \leq 1000 \\
0.424 & \text{for } \text{Re}_d > 1000
\end{cases},
\]

with \( \text{Re}_d = \rho_g \hat{u}_{\text{rel}} d / \mu_g \), where \( \hat{u}_{\text{rel}} = |\hat{u}_g - \hat{u}_l| \) is the relative velocity and \( \mu_g \) the molecular viscosity of the gas-phase mixture.

2.4. Droplet Breakup Model

The primary breakup of the liquid jet was not modeled in the original CAS model. Instead, an initial droplet size of \( \sqrt{0.1 \times D^2} \) was set at the nozzle exit, after studying sensitivity of liquid penetration. The Reitz and Diwakar (1986) (RD) wave breakup model was used for the secondary breakup, assuming that most breakups were of stripping-type (Reitz, 1987) (see Appendix A). In this work, a combined Kelvin-Helmholtz (KH) / Rayleigh-Taylor (RT) breakup model (Patterson and
Reitz, 1998) was incorporated. Under the monodispersed droplet assumption, an equation for the transport of droplet diameter is solved, which is an extension of the well-known $d^2$-law. The droplet breakup source term is computed as $\dot{\omega}_{\text{bre}} = K_{\text{bre}} \dot{\rho} \dot{Y}_1$, where the breakup coefficient, $K_{\text{bre}}$, is modeled as

$$K_{\text{bre}} = \frac{2\dot{d}(\dot{d} - d_{\text{st}})}{\tau_b}, \quad (17)$$

The stable droplet diameter ($d_{\text{st}}$) and breakup time ($\tau_b$) are computed from either the KH or the RT breakup model, depending on the local breakup length and time scales of the corresponding models:

$$d_{\text{st}, \text{KH}} = 2B_0 \Lambda_{\text{KH}}, \quad (18)$$

$$\tau_{b, \text{KH}} = 3.788B_1 \frac{\dot{d}}{2\dot{\Lambda}_{\text{KH}} \Omega_{\text{KH}}}, \quad (19)$$

$$d_{\text{st}, \text{RT}} = C_3 \Lambda_{\text{RT}}, \quad (20)$$

$$\tau_{b, \text{RT}} = \Omega_{\text{RT}}^{-1}. \quad (21)$$

Details on the calculation of the growth rate, $\Omega$, and the corresponding wavelength, $\Lambda$, of the fastest growing wave are not given here for brevity and can be found in Patterson and Reitz (1998). The original formulation of the RT model generates multiple droplets at the end of the breakup time. However, in this work, an approach of the continuous breakup is followed for simplicity, which is similar to the KH model and results in a continuous decrease of the droplet diameter. The first, near-nozzle breakup is always modeled by the KH model. Modeling of subsequent breakup events is decided based on the corresponding stable diameter and breakup time from the respective models. If the current droplet diameter is larger than $d_{\text{st}, \text{RT}}$ and $\tau_{b, \text{RT}} < \tau_{b, \text{KH}}$, the RT model is used; otherwise, the breakup occurs through the KH model. No breakup happens if both $d_{\text{st}, \text{KH}}$ and $d_{\text{st}, \text{RT}}$ are larger than the current droplet diameter.

For different nozzles, the breakup model constants $C_3$ in Eq. (20) for the RT model or $C_b$ in Eq. (A.10) for the Reitz-Diwakar model need to be tuned to match the experimental liquid length. This is reasonable because the internal nozzle flow can have a significant effect on the primary breakup (Han et al., 2002; Gorokhovski and Herrmann, 2008; Som et al., 2011; Agarwal and Trujillo, 2020). The standard ranges of values for the model constants are reported in Table 1, along with the values used in this work. Although Patterson and Reitz (1998) suggested a range of 1.0-5.33 for $C_3$, Bravo and Kweon (2014) and Wehrfritz et al. (2012) have used $C_3$ of 0.1 for evaporating sprays in their simulations. In summary, these constants depend on the nozzle geometry and therefore are tuned for a given injector nozzle. Once tuned for an injector, the model can be used for any operating condition or fuel without any further tuning.
| Model                  | Constant | Standard range | Present work |
|-----------------------|----------|----------------|--------------|
| Kelvin-Helmholtz      | $B_0$    | 0.61           | 0.61         |
|                       | $B_1$    | 1.73-60.0      | 10.0         |
| Rayleigh-Taylor       | $C_3$    | 0.1-5.33       | Spray A: 0.60 |
|                       |          |                | Spray C: 0.80 |
|                       |          |                | Spray D: 0.85 |
|                       |          |                | FSC: 0.75    |
| Reitz-Diwakar         | $C_b$    | 10.0           | Spray A: 10.0 |
|                       |          |                | Spray C: 10.0 |
|                       |          |                | Spray D: 12.0 |
|                       |          |                | FSC: 12.0    |

Table 1: Breakup model constants.

2.5. Droplet Size Distribution

The mean droplet size along the axis provides little information regarding the distribution of sizes. Early studies of diesel sprays have shown the droplet size distributions to be highly skewed, which can be represented by Rosin and Rammler (1933), logarithmic normal (Mugele and Evans, 1951), Nukiyama and Tanasawa (1939), or Chi-square distributions (Hiroyasu and Kadota, 1974). In recent investigations, lognormal distributions were found to be suitable for diesel sprays (Feng et al., 2019).

We extended the CAS model to consider the droplet size distribution. In this case, the droplet size distribution is modeled as a two-parameter presumed probability distribution function (PDF), which can be fitted with parameters depending on moments of droplet diameter. Droplets of all sizes are assumed to be at the local mean droplet temperature ($\hat{T}_d$). The terms dependent on droplet diameters are then integrated over the presumed PDF. The original CAS equation already contained an equation for the second moment of the diameter. Additionally, we derived the equation for the first moment or mean of the droplet diameter. The presumed PDFs are modeled as one of the Rosin-Rammler, lognormal, and gamma distribution functions and used as the boundary condition at the nozzle exit. Table 2 shows the PDFs and their moments, which can be used to fit the parameters $m$ and $n$. For lognormal and gamma distributions, closed expressions can be obtained for the parameters as a function of the first and second moments of droplet diameters. However, this is not possible for the Rosin-Rammler distribution, and therefore, the parameters, $m$ and $n$, are computed iteratively. The current limitation of this approach is that the initial droplet size distribution at the nozzle exit must
be known either from measurements or primary breakup DNS; otherwise only the delta PDF can be used, which leads to the blob injection model (Reitz, 1987; Reitz and Diwakar, 1987).

| PDF          | \( \mathcal{P}(\hat{d}) \) | \( \langle \hat{d} \rangle \) | \( \langle \hat{d}^2 \rangle \) |
|--------------|-------------------------------|-----------------------------|-----------------------------|
| Rosin-Rammler | \( \frac{m}{n} \left( \frac{d}{\hat{d}} \right)^{m-1} \exp \left( - \left( \frac{d}{\hat{d}} \right)^{m} \right) \) | \( n \Gamma \left( 1 + \frac{1}{m} \right) \) | \( n^2 \Gamma \left( 1 + \frac{2}{m} \right) \) |
| Log-Normal   | \( \frac{1}{dn \sqrt{2\pi}} \exp \left( - \frac{(\ln(\hat{d}) - m)^2}{2n^2} \right) \exp \left( m + \frac{n^2}{2} \right) \exp(n^2) \exp \left( 2m + n^2 \right) \) | \( \frac{n \Gamma(m) \hat{d}^{m-1} \exp(-n\hat{d})}{m} \) | \( \frac{m(m+1)}{n^2} \) |
| Gamma        | \( \frac{n^m}{\Gamma(m)} \hat{d}^{m-1} \exp(-nd) \) | \( \frac{m}{n} \) | \( \frac{m(m+1)}{n^2} \) |
| Delta        | \( \delta(\hat{d}' - \hat{d}) \) | \( \hat{d} \) | \( \hat{d}^2 \) |

Table 2: Presumed PDFs to model the droplet size distribution.

2.6. Transport of Vapor Mass Fraction

The original CAS model did not track the vapor mass fraction explicitly. Therefore, the far-field vapor mass fraction was assumed to be zero in the evaporation model. While this assumption can be a good approximation for a fast-mixing turbulent spray, it may lead to errors in the calculation of mass transfer number, which may overestimate the evaporation rate and reduce the liquid length. Therefore, an explicit transport equation (Eq. (4)) is proposed for the vapor mass fraction by splitting the original gas phase continuity equation Eq. (A.1). The source terms, \( \dot{\omega}_{\text{ent},a} \) and \( \dot{\omega}_{\text{vap}} b^2 \), are mutually exclusive as the entrainment brings purely ambient gas into the spray plume and the evaporation brings pure vapor from the liquid phase into the gas phase. In the gas phase, both ambient gas and fuel vapor are assumed to be perfectly mixed.

2.7. Evaporation and Droplet Heating Model

The original CAS model used the correlations by Frössling (1938) to model evaporation from the external droplet surface. In this work, we applied the evaporation model of Miller and Bellan (1999), which contains a non-equilibrium treatment of the vapor mass fraction on the droplet surface. The evaporation source term is computed as

\[
\dot{\omega}_{\text{vap}} = \frac{3K_{\text{vap}} \bar{\rho} Y_i}{2\hat{d}^2},
\]

where

\[
K_{\text{vap}} = 4\frac{\rho_e}{\rho_l} \Gamma_{\text{v,e}} \ln(1 + B_{M,d}) \text{Sh}_d.
\]
The diffusion coefficient of fuel vapor (subscript ‘v’) in the surrounding gas mixture. The droplet mass transfer number is defined as

$$B_{M,d} = \frac{Y_{v,s} - Y_{\infty,v}}{1 - Y_{v,s}},$$

where the non-equilibrium vapor mass fraction on the droplet surface is modeled as

$$Y_{v,s} = \frac{\chi_{neq,v,s}}{\chi_{neq,v,s} + (1 - \chi_{neq,v,s})WR},$$

where $WR = W_a/W_f$ is the ratio of the molecular weight of the ambient gas excluding vapor (subscript ‘a’) to the molecular weight of fuel (subscript ‘f’). The subscript ‘s’ denotes variables at the droplet surface. The non-equilibrium vapor mole fraction, $\chi_{neq,v,s}$, at the droplet surface is obtained as

$$\chi_{neq,v,s} = \chi_{eq,v,s} - \left(\frac{2L_{Kn}}{d}\right)\xi.$$

Miller and Bellan (1999) proposed the Clausius-Clapeyron relation to obtain equilibrium molar fraction, $\chi_{eq,v,s}$. However, a reasonable calculation of $\chi_{eq,v,s}$ requires appropriate reference values of saturation temperature and pressure. Since the vapor pressure is directly available from the fuel properties, the equilibrium vapor mole fraction, $\chi_{eq,v,s}$, at the droplet surface is computed as

$$\chi_{eq,v,s} = \frac{p_v(T_d)}{P_g},$$

where $P_g$ is ambient gas pressure and $p_v(T_d)$ the vapor pressure at the droplet temperature. The molecular Knudsen layer thickness, $L_{Kn}$, is computed as

$$L_{Kn} = \frac{\mu_a \left(2\pi T_d R/W_v\right)^{1/2}}{Sc_g P_g},$$

whereas the non-dimensional evaporation parameter, $\xi$, is given by

$$\xi = \frac{1}{2} \frac{Pr_g}{Sc_g} \ln(1 + B_{M,d})Sh_d.$$

It is noted that the parameter $\xi$ requires implicit calculations. As reported by Miller and Bellan (1999), $\xi$ is a slowly varying parameter and constant for droplets following the ‘$d^2$-law’. As a consequence, it is not necessary to perform iterative calculations, and the value from the previous iteration can be used. In this work, the following procedure is used:

1. The value of $B_{M,d}$ is computed from the equilibrium $Y_{v,s}$ using Eq. (A.14),
2. The initial value of $\xi$ is calculated,
3. $\chi_{neq,v,s}$ is computed using Eq. (26) and $Y_{v,s}$ using Eq. (25),
4. $B_{M,d}$ is then updated using the non-equilibrium $Y_{v,s}$. 

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5. ξ is updated.

The far-field vapor mass fraction, \( Y_{∞,v} \), in the calculation of the mass transfer number Eq. (24) is set according to the one-third rule (Hubbard et al., 1975) to \( Y_{∞,v} = C_{vap}(\hat{Y}_v + 2Y_{v,s})/3 \). An additional scaling constant, \( C_{vap} = b(0, t)/b(z, t) \), is introduced to account for the effects of locally entrained fresh ambient gas encountered by droplets away from the centerline. Differently, in the original CAS model, \( \hat{Y}_v \) was set to zero assuming the far-field value of the vapor mass fraction to be negligible.

The droplet temperature is affected by continuous heating and evaporation. The respective source term is modeled as \( \dot{\omega}_{\text{heat}} = K_{\text{heat}} \tilde{\rho} \hat{Y}_l \) with the temperature coefficient, \( K_{\text{heat}} \), given by

\[
K_{\text{heat}} = \frac{6Q_d}{\rho_d C_l(T_d)} - \frac{3K_{vap}L(\hat{T}_d)}{2d^2C_l(T_d)},
\]

where \( L(\hat{T}_d) \) and \( C_l(\hat{T}_d) \) are the latent heat of vaporization and the heat capacity of the fuel at the droplet temperature \( \hat{T}_d \), respectively. The heat transfer between the droplet and ambient gas mixture is modeled as

\[
Q_d = \frac{\lambda_g(T_{\text{rel}})(\hat{T}_g - \hat{T}_d)}{d} f_2 \text{Nu}_d,
\]

where \( \lambda_g(T_{\text{rel}}) \) is the thermal conductivity of the local gas-phase mixture and \( \hat{T}_g \) the ambient gas temperature. Since the vapor mass fraction is now known, \( \hat{T}_g \) can be computed assuming homogeneous mixing of vapor in the ambient gas as

\[
\hat{T}_g = \frac{\hat{Y}_v \hat{T}_v + \hat{Y}_a \hat{T}_a}{\hat{Y}_g},
\]

where the vapor temperature \( \hat{T}_v \) is calculated iteratively from the droplet temperature by using the latent heat of vaporization for evaporation. The analytical evaporative heat transfer correction, \( f_2 \), is given by

\[
f_2 = \frac{\xi}{e^\xi - 1}.
\]

For completeness, the correlations for the droplet Sherwood and Nusselt numbers from Ranz and Marshall (1952) are given here:

\[
\text{Sh}_d = 2 + 0.552 \frac{1}{2} \text{Re}_d^{1/2} \text{Sc}_g^{1/3},
\]

\[
\text{Nu}_d = 2 + 0.552 \frac{1}{2} \text{Pr}_g^{1/3}.
\]

The gas-phase Schmidt number, \( \text{Sc}_g \), is defined as

\[
\text{Sc}_g = \frac{\mu_g}{\rho_g \Gamma_{v,g}}
\]
and the gas-phase Prandtl number, $Pr_g$, is defined as

$$Pr_g = \frac{\mu_g(T_{ref})C_{p,g}(T_{ref})}{\lambda_g(T_{ref})}.$$  \hfill (37)

$C_{p,g}(T_{ref})$ is the specific heat capacity of the gas-phase mixture at constant pressure, which is computed by the linear mixing rule as

$$C_{p,g} = \frac{\hat{Y}_v C_{p,v} + \hat{Y}_a C_{p,a}}{\hat{Y}_g}.$$  \hfill (38)

The gas-phase mixture properties and correlations are computed at the reference temperature, which is obtained by the one-third rule (Hubbard et al., 1975) as

$$T_{ref} = \frac{\hat{T}_g + 2\hat{T}_d}{3}.$$  \hfill (39)

Since the boiling model is not used, the droplet temperature is kept bounded by an upper limit of saturation temperature at the given pressure. The liquid properties such as density ($\rho_l$), surface tension ($\sigma_l$), and viscosity ($\mu_l$) are evaluated at a constant fuel temperature at the nozzle exit ($T_{l,o}$) and remain constant throughout the liquid phase. The gas-phase mixture properties, such as viscosity ($\mu_g$) and thermal conductivity ($\lambda_g$), are computed from the vapor and ambient gas properties by Wilke (1950) formula.

2.8. Nozzle Flow Model

In the original CAS model, injection velocities were computed using simple Bernoulli relations considering the measured discharge coefficient ($C_D$). In this work, a phenomenological zero-dimensional nozzle flow model from von Kuensberg Sarre et al. (1999) is used to predict the nozzle exit velocity. The initial nozzle exit velocity is computed from Bernoulli’s equation, assuming the discharge coefficient of unity. The discharge coefficient is then computed iteratively using a correlation based on inlet and expansion losses. The final mean exit velocity is computed from the converged value of the discharge coefficient. The nozzle flow model provides the effective jet velocity and effective jet diameter, which can be different from the geometric nozzle exit diameter if cavitation or hydraulic flip occur within the nozzle.

2.9. Numerical Methods

The hyperbolic system of PDEs Eq. (3)-(10) is numerically solved in conservative form. An upwind convective scheme is required to account for the possible discontinuities in the multiphase system. Wan (1997) used a combination of Beam and Warming (1976) and MacCormack (1969) schemes to avoid oscillations in the solution. In this work, various numerical schemes such as first order
Lax-Friedrichs (Lax, 1954) and the third and fifth order weighted essentially non-oscillatory (WENO) schemes (Jiang and Shu, 1996) are implemented. Numerical tests did not show significant benefit in the accuracy of quantities of interest with higher order schemes. Therefore, the Lax-Friedrichs scheme employing Rusanov fluxes (Rusanov, 1961) with local wave speeds is chosen to keep computational costs low. An explicit Euler scheme is used for the time advancement. Since different physical processes, which are lumped together in the source terms, have different time scales, a Courant-Friedrichs-Lewy (CFL) number of 0.1-0.5 is used to ensure stability. The governing equations and models are implemented in an in-house FORTRAN code framework, named CARTS.

2.10. Solution Procedure

The variables in the governing equation are non-dimensionalized using the effective jet diameter $D_0$ as the length scale, the effective jet velocity $U_0$ computed using nozzle flow model in Subsection 2.8 as the velocity scale, and $\tau_0 = D_0/U_0$ as the time scale. The mixture density and temperatures are non-dimensionalized by the liquid phase density ($\rho_l$) and nozzle exit temperature ($T_{1,o}$), respectively. The non-dimensional (ND) system of equations is discretized in space and time, the variables are initialized in the 1D discretized domain, and boundary conditions (BCs) are applied with the left boundary as the liquid jet and the right boundary treated as the far-field condition. The initial (IC) and boundary conditions of the ND variables are given in Table 3. First, the conservative ND variables are advanced in time. The primitive ND variables are then computed from the conservative ND variables. Numerical difficulties occur when liquid- or gas-phase mass fractions become small. A threshold of $10^{-6}$ for the liquid phase mass fraction, $Y_l^*$, produces a numerically stable solution. Below this threshold, all liquid phase variables are set to zero. In addition, the summation of mass fractions is ensured to be unity, adjusting the value of the ambient gas mass fraction ($Y_a^*$). The primitive variables are bounded by their physical limits to avoid an unphysical solution. For the cases with droplet size distribution, the droplet diameters are discretized into a fixed number (in this work, 200) of classes about the mean diameter to represent the PDF.

3. Description of Cases and Validation Data

3.1. ECN Data

Selected experimental data from the Engine Combustion Network ECN (2020) are used for validation of the model under a wide range of operation conditions. The initial and boundary conditions corresponding to the measurement data of the selected inert inert cases are summarized in Table 4 (cases 1-11). A detailed description of the cases and the measurement setup can be found on the ECN webpage (ECN, 2020) and in previous literature (Pickett et al., 2010, 2011; Skeen et al., 2015).
shows the geometric details and the hydraulic coefficients of the nozzles considered in this work. The rate of injection is generated using the virtual injection rate generator (Payri et al., 2020).

### 3.2. FSC Data

In addition to the ECN data, the data generated within the FSC are used (cases 12-15) to evaluate the model for the effect of different fuel properties. The data have been measured in a pressure chamber, which is built as a heated constant-pressure optically accessible flow vessel (ambient gas velocity, \( u_a \leq 0.1 \text{ m/s} \)). Ambient conditions up to 835 K and 50 bar are presented. The 8-hole injector is centrally positioned in the chamber so that one of the spray plumes propagates vertically from bottom to top, which is then investigated. The fuel is provided by a common-rail injection system with a maximum investigated injection pressure of 1400 bar.

For measuring the liquid penetration, Mie scattering visualizations were used, while the Schlieren technique was used for determining vapor penetration. The optical access of the pressure vessel limits the maximum detectable spray penetration to 55 mm. To determine the vapor penetration and cone angles in the Schlieren images, the spray must be separated from the surrounding gas phase to guarantee a valid binarization. A Gaussian Fast Fourier Transformation Filter is used to suppress the different textures/frequencies of the surrounding ambience. Afterwards, the post-processing procedure for the

| Variable | Definition | IC | Left BC | Right BC | Bounds |
|----------|------------|----|---------|----------|--------|
| \( Y_1^* \) | \( \hat{Y}_1 \) | 0.0 | Dirichlet 1.0 | Neumann 0.0 | [0.0,1.0] |
| \( Y_2^* \) | \( \hat{Y}_2 \) | 0.0 | Dirichlet 0.0 | Neumann 0.0 | [0.0,1.0] |
| \( Y_3^* \) | \( \hat{Y}_3 \) | 1.0 | Dirichlet 0.0 | Neumann 0.0 | [0.0,1.0] |
| \( \rho^* \) | \( \hat{\rho}/\rho_l \) | \( \rho_a/\rho_l \) | Dirichlet 1.0 | Neumann 0.0 | [\( \rho_l/\rho_l \),1.0] |
| \( u_i^* \) | \( \hat{u}_i/\bar{U}_o \) | 0.0 | Dirichlet 1.0* | Neumann 0.0 | [0.0,1.0] |
| \( u_g^* \) | \( \hat{u}_g/\bar{U}_o \) | 0.0 | Dirichlet 0.0 | Neumann 0.0 | [0.0,1.0] |
| \( \langle d'^2 \rangle \) | \( \langle \hat{d}^2 \rangle/D_o^2 \) | 0.0 | Dirichlet 0.1-1.0 | Neumann 0.0 | [0.0,1.0] |
| \( \langle d' \rangle \) | \( \langle \hat{d} \rangle/D_o \) | 0.0 | Dirichlet 0.1-1.0 | Neumann 0.0 | [0.0,1.0] |
| \( T_d^* \) | \( \hat{T}_d/T_{l,o} \) | 0.0 | Dirichlet 1.0 | Neumann 0.0 | [0.0,T_{sat}/T_{l,o}] |
| \( T_g^* \) | \( \hat{T}_g/T_{l,o} \) | \( T_{amb}/T_{l,o} \) | Neumann 0.0 | Neumann 0.0 | [0.0,T_{amb}/T_{l,o}] |
| \( b^* \) | \( \hat{b}/D_o \) | 0.5 | Dirichlet 0.5 | Neumann 0.0 | [0.5,\infty) |
| \( z^* \) | \( \hat{z}/D_o \) | - | 0.0 | 1600.0 | [0.0,1600.0] |
| \( t^* \) | \( \hat{t}/\tau_o \) | 0.0 | - | - | [0.0,\infty) |

Table 3: Initial and boundary conditions.*Normalized rate of injection profile is applied, if available.
Table 4: Cases chosen for validation in this study. *Measured vapor cone angle. **Computed by Eq. (13). Breakup model constants $C_b$ and $C_3$ were tuned for injector nozzles for cases 1, 10, 11, and 12.

Mie-scattering based on background subtraction and a fixed intensity threshold for binarization can be applied to the filtered Schlieren images. Only the first half of the spray is considered to measure the steady-state cone angles, which are not influenced by entrained air (Naber and Siebers, 1996). Fuel injections were repeated 20 times with a frequency of 0.2 Hz. A detailed description of the performed measurements can be found in Palmer et al. (2015).

The measured vapor cone angles and the spray cone angles computed by Eq. (13) are reported in Table 4 for comparison. The rate of injection was not measured. Therefore, appropriate linearly increasing rate of injection profiles were used to closely reproduce initial stages of the spray evolution as observed in the experiments.

### 3.3. Simulation Data

Additional validation is performed with the results of a 3D LES as well as unsteady RANS (URANS) simulations as reference and benchmark for the 1D model. The LES was performed using an in-house
| Parameter                          | Symbol | Unit | Spray A | Spray C | Spray D | FSC |
|-----------------------------------|--------|------|---------|---------|---------|-----|
| # of holes                        | -      | -    | 1       | 1       | 1       | 8   |
| Sac diameter                      | \(D_{\text{sac}}\) | \(\mu m\) | 660     | 660     | 2500*   | 124 |
| Exit diameter                     | \(D_{\text{noz}}\) | \(\mu m\) | 90      | 200     | 189     | 109 |
| Inlet radius to exit diameter ratio | \(r/D_{\text{noz}}\) | -    | 0.256   | 0.2     | 0.55    | 0.125 |
| Length to exit diameter ratio     | \(L_{\text{noz}}/D_{\text{noz}}\) | -  | 11      | 5       | 5.5     | 9.4  |
| Inlet loss coefficient            | \(K_{\text{in}}\) | -    | 0.035   | 0.039   | 0.039   | 0.085 |
| Expansion loss coefficient        | \(K_{\text{exp}}\) | -    | 0.0     | 0.0     | 0.0     | 0.01 |
| Discharge coefficient (measured)  | \(C_D\) | -    | 0.89    | -       | -       | 0.86-0.91 |
| Discharge coefficient (computed)  | \(C_D\) | -    | 0.89    | 0.95    | 0.94    | 0.87-0.90 |

Table 5: Geometric and hydraulic parameters for different nozzles. *Sac diameter for Spray D is increased from 660 \(\mu m\) to obtain a reasonable cone angle through the model.

The commercial 3D CFD software CONVERGE from Convergent Science Inc. (Richards et al., 2017) was employed for the URANS simulation of the Spray A case under inert conditions. The Spray A case has been widely studied using CONVERGE (Senecal et al., 2014; Wang et al., 2014). The URANS simulations in this work used the base grid size of 1.5 mm with near-nozzle fixed embedding to level 3, resulting in the smallest grid size of 0.1875 mm. Adaptive mesh refinement (AMR) up to
level 3 was used outside the fixed embedding, which enabled local refinement depending on the flow conditions. This resulted in the cell count varying in the range of $3 \times 10^5$ to $1.2 \times 10^6$. The KH-RT breakup model and Frössling (1938) evaporation model were used in the simulation.

The differences in physical models and parameters between the 3D CFD model and the 1D CAS model are noted. Simpler physical models in the CAS model reduce the computational costs and therefore are preferred. For example, while URANS used the dynamic drag model, the spherical drag model was used in the LES and CAS model. Similarly, the collision model was not used in the LES and CAS model. In 3D CFD, droplet breakup and evaporation result in droplets of various sizes at each axial location, whereas in the CAS model, the droplets are either assumed to be monodispersed across the cross-section or presumed PDFs are used to represent the local droplet size distribution as described in Subsection 2.5. Due to Lagrangian-Eulerian approach in the 3D simulations, the mixture density does not contain contributions from the liquid phase. Therefore, the density-weighted cross-sectional averages of the available flow variables were computed differently compared to those defined by Eq. (1). The boundaries of the spray plume were first determined by the threshold vapor mass fraction of 0.035. Within the spray boundaries, the averages of the flow variables were then computed. The threshold value was entered by a visual inspection of the spray plume, as lower values resulted in excessive dilution of the flow variables by their far-field values.

4. Results and Discussion

The solution of the governing equations of the CAS model provides flow variables such as density, mass fractions and velocities of the liquid and vapor phases, mean droplet diameter, and the droplet temperature along the axial co-ordinate. From these data, the global spray characteristics such as liquid and vapor penetration were extracted. The ECN guidelines suggest the liquid penetration length to be determined as the farthest axial location from the nozzle exit where the liquid volume fraction is 0.1\%, and the vapor penetration length to be determined as the farthest axial location from the nozzle exit where the vapor mass fraction is 0.1\%. Since the vapor mass fraction is not explicitly tracked in the original CAS model, the vapor or gas penetration is determined as the axial location from the nozzle exit where the gas velocity normalized by the nozzle exit velocity ($U_o$) is 0.1\%. This definition was found to be equivalent to that of the ECN. First, the original CAS model was evaluated for a wide range of conditions and fuels. The incremental improvements in the model performance are then discussed, as the new sub-models are added or replaced.

4.1. Grid Convergence

A grid convergence study was performed with the original CAS model to select the grid size for further computations. Figure 1a shows the effect of increasing grid resolution on the liquid and vapor
penetration for the Spray A case 1. The grid resolution is represented in terms of the effective jet diameter \((d_z = p \times D_o)\). Both liquid and vapor penetration converge as the grid size is decreased. From this study, the grid size of \(1 \times D_o\) was chosen as a compromise between accuracy and computational cost, and the simulations reported in the following subsections were performed with this chosen grid size.

4.2. Initial Droplet Size

In the original CAS model, the initial droplet size of \(\sqrt{0.1 \times D_o^2}\) was suggested. In this work, various initial droplet sizes were tested to evaluate their effect on the liquid and vapor penetration lengths. Results in Figure 1b (for Spray A case 1) show a significant effect of the initial droplet size on the liquid penetration, whereas the vapor penetration is hardly affected, except in the initial phase before 0.2 ms. The sensitivity to the initial droplet size was also verified for other selected cases, but results are not shown here for brevity. The initial droplet size of \(\sqrt{1 \times D_o^2}\) can predict the liquid and vapor penetration reasonably well, and therefore it was used for all cases in this work. This corresponds to the blob injection model (Reitz, 1987; Reitz and Diwakar, 1987).

4.3. Results with the Original CAS Model

For validation, the liquid and vapor penetration lengths for case 1 with inert ambient conditions are compared in Figure 2. The liquid penetration length from CAS agrees well with URANS, LES,
and the experimental values. The vapor penetration length from the CAS model agrees well with the measurements. While LES predicts the vapor penetration quite well, the URANS results deviate from the experiments after approximately 0.7 ms. Such deviations have also been observed in Senecal et al. (2014) in the grid-converged results. The results of the URANS simulations performed in this work are close to the converged values with the finer resolution in their grid convergence study. Despite model reductions, the 1D CAS model captures the vapor length closely. The reasons for such agreement can be attributed to the strong dependency on the initial momentum and correct momentum transfer from the liquid to the gas phase due to the Eulerian description. Previous studies have shown that incorrect coupling between the liquid and gas phases can occur in Lagrangian particle tracking methods, and thus spray penetration can become highly grid-dependent (Abraham, 1997; Béard et al., 2000; Post et al., 1999; Qiu and Reitz, 2015; Wei et al., 2017). In the recent studies, Eulerian spray models have been able to correctly reproduce the vapor penetration in URANS (Garcia-Oliver et al., 2013; Blanco, 2016) and LES (Matheis and Hickel, 2018; Desantes et al., 2020). Another factor affecting vapor penetration is the turbulence model, which has an influence on the entrainment of ambient gas. Studies have shown the RANS models to underpredict the vapor penetration at longer times, while the LES results always matched the measurements well (Zhou et al., 2011; Xue et al., 2013; Kahila et al., 2018). The entrainment of the ambient gas in the CAS model comes through the spreading of the spray specified by the spray angle and implicitly considers the turbulence effects.

![Figure 2: Comparison of the liquid and vapor penetration lengths in the LES, the URANS simulation, and the CAS model for case 1.](image)

The original CAS model is then applied to ECN cases (2-11) from Table 4, and the performance of the model is analyzed with respect to varying ambient pressures (or densities), injection pressures, ambient temperatures, and nozzles. Experimental data are shown where available. The effects of ambient pressure (or density) on spray penetration are well-known from previous studies (Naber et al., 1995; Siebers, 1998, 1999), where a strongly non-linear trend of the liquid and vapor lengths with
Figure 3: Effect of ambient pressure, injection pressure, nozzle geometry, and ambient temperature on the liquid and vapor penetration lengths (cases 1-11).
respect to ambient pressure has been reported. This effect is reproduced well by the model, as shown in Figure 3(a). The variation of injection pressure has a primary effect on the vapor penetration but no observable effect on the liquid penetration (see Figure 3(b)), which is also captured well by the model. The injection pressure directly controls the momentum flux at the nozzle exit, which has an impact on the vapor penetration, or in other words, the spray tip penetration. On the other hand, the liquid penetration is governed by breakup and evaporation processes, which are not significantly changing as the injection pressures are sufficiently high.

Figure 3(c) shows the effect of different nozzles. For different nozzles, the breakup model constant $C_b$ in Eq. (A.10) needed to be tuned to match the experimental liquid length as discussed in Section 2.4. It includes the effects of the internal nozzle flow on the primary breakup. While the recommended value of 10.0 for $C_b$ was used for Spray A and Spray C, it was increased to 12.0 for Spray D. For these cases, the results cannot be considered as validation. However, it must be noted that the values of model constants are calibrated only once for a given injector. Once tuned, the model should be expected to produce reasonable trends in liquid and vapor lengths for a wide range of operating conditions and fuels.

Figure 3(d) shows the effect of varying ambient temperatures on spray characteristics. The vapor penetration is affected less by ambient gas temperatures compared to the liquid penetration. On the other hand, the liquid length decreases with increasing gas temperature as observed in the measurements. The model is not able to predict these trends in liquid length with respect to the gas temperature.

The model is then applied to FSC cases (12-15) with two different fuels, namely 1-octanol and di-$n$-butylether (dnbe), and two different ambient conditions (see Figure 4). For both conditions, the liquid length for 1-octanol is higher because of higher heat of vaporization (see Figure 5(a)) and lower vapor pressure (see Figure 5(b)) in comparison with di-$n$-butylether. The model is not able to bring these differences in the fuel properties into the liquid lengths of the two fuels. Similar to Spray D, the value of $C_b$ was set to 12.0 for the FSC nozzle.

4.4. Results with Model Improvements

The CAS model, in its original formulation, can reasonably predict the effects of ambient pressure, injection pressure, and nozzle geometry on liquid and vapor penetration of sprays. However, it fails to capture the effect of ambient temperature and, more importantly, the effect of fuel properties, as discussed in the previous section. Therefore, the model was improved in its predictive capabilities by updating the current standard breakup and evaporation models, as described in Section 2. In addition, a transport equation of vapor mass fraction was added.
Figure 4: Effect of different fuel properties on the liquid and vapor penetration lengths (cases 12-15).

Figure 5: Selected properties of 1-octanol and di-n-butylether (Daubert and Danner, 1989).

4.4.1. KH-RT Breakup Model

The simulations for all cases (1-15) were performed with the combined KH-RT breakup model. For brevity, the results are reported here only for the cases showing significant deviations from the trends. Figure 6(a) shows the results for varying ambient temperatures. With increasing ambient temperature, the liquid penetration should decrease as observed in the experiments. This trend is followed for
temperatures from 440 K to 900 K. For the temperature of 440 K, there is no clear distinction between liquid and vapor penetration, which is consistent with the measurements. However, for the temperature of 1200 K, the predicted liquid penetration is not consistent with the trend and measurements.

Compared to the Reitz-Diwakar breakup model, the combined KH-RT breakup model captures the effects of different fuel properties to a certain extent, as shown in Figure 6(b). However, the predicted liquid lengths are lower than those measured for both fuels.

4.4.2. Transport of Vapor Mass Fraction

Figure 7 shows the results for varying ambient temperatures and different fuels with the additional information on the vapor mass fraction. The trends in the temperature variation are improved significantly, particularly for the case at the temperature of 1200 K. However, the liquid penetration for the temperature of 700 K is slightly lower. On the other hand, no particular benefit is observed in the liquid lengths of 1-octanol and di-n-butylether, which are still underpredicted.

4.4.3. Evaporation Model from Miller and Bellan

The upgrade of the evaporation model to that of Miller and Bellan (1999) concludes the improvements in the monodisperse CAS model. For completeness, the results for all cases (1-15) are shown
in Figures 8 and 9. Figure 8(d) shows the improvements in the liquid length for the ambient temperatures of 700 K and 900 K. The model prediction of the liquid penetration for di-n-butylether and 1-octanol has improved significantly (see Figure 9) at both operating conditions.

The liquid penetration from the CAS model shows a jump (e.g., in Figure 9), which can be understood by observing the volume fraction of the liquid phase because the liquid length is determined as the farthest location from the nozzle exit where the liquid volume fraction falls below 0.1 %. Figure 10 shows the successive liquid volume fraction profiles along the axis of the spray for case 12 as an example. The localized bump at the tip of the spray is formed due to the initial transient ramp of the needle motion. As the initial velocity of the jet is lower than the steady-state velocity, breakup and evaporation of the large liquid mass are slow in the beginning. At the steady-state injection rate, the bump gradually flattens, and the liquid length jumps to lower values as soon as the bump falls below the threshold of 0.1 %.

4.5. Comparison with Simulation Data

In addition to validation with the experimental data, the improved CAS model is compared in detail with the LES and URANS results. Figure 11 shows the non-dimensional flow variables from the
Figure 8: Results using the KH-RT breakup model, the transport equation for the vapor mass fraction, and the evaporation model of Miller and Bellan for cases 1-11.
Figure 9: Results using the KH-RT breakup model, the transport equation for the vapor mass fraction, and the evaporation model of Miller and Bellan for cases 12-15.

Figure 10: Liquid volume fraction at successive times (left), zoomed view (right) for case 12. Horizontal dashed gray line indicates the criterion of the liquid volume fraction ($\alpha_l$) = 0.1% for the liquid penetration length.

CAS model, the URANS simulation, and the LES along the non-dimensional axial coordinate (defined in Table 3). The two-phase mixture density ($\rho^*$), mass fractions of the liquid ($Y_l^*$) and the ambient gas ($Y_a^*$), and velocity of the liquid phase ($u_l^*$) and the gas phase ($u_g^*$) along the axial coordinate are shown in Figure 11(a). Due to the Lagrangian description, all variables are not directly comparable with those from the LES and URANS simulations.
Figure 11: Comparison of non-dimensional flow variables predicted with the CAS model and the URANS simulation at $t = 1 \text{ ms}$ and the time-averaged LES for case 1.

The gas-phase mixture fraction (or vapor mass fraction in the inert case) is available in the ECN experimental data, the URANS results, and the LES results for comparison. Its cross-sectional average is compared with the mixture fraction from the CAS model (see Figure 11(b)). Until $t = 1 \text{ ms}$, the vapor in the URANS simulation has traveled to a shorter distance compared to the LES as well as the CAS model, which is consistent with the lower penetration length observed in the URANS simulation in Figure 2. In the LES, the values are averaged in time during the steady-state phase from $t = 1 \text{ ms}$ to $2 \text{ ms}$. All of the simulation models are able to reasonably represent the mixture fraction away from the nozzle, although there are differences near the nozzle. The results of the CAS model are closer to the URANS results rather than the LES results, as expected given the averaged approach of the CAS model.

Figure 11(c) shows the mean droplet diameters along the axis of the spray from the LES, URANS, and CAS models. In the LES, the mean droplet diameter drops rapidly within a distance of $\approx 10D_{\text{noz}}$. In contrast, the mean droplet diameter in the URANS simulation decreases gradually over the liquid length. The mean droplet diameter in the CAS model shows trends similar to the LES but different from URANS, although a very similar KH-RT breakup model is used in all simulation approaches.

The mean droplet temperature in the CAS model follows the URANS result closely near the nozzle
exit but deviates at farther distances, as shown in Figure 11(d). On the other hand, the droplets in the LES are heated much faster close to the nozzle, as the mean droplet diameter is much smaller compared to other simulation models. After $\approx 10D_{noz}$, the mean droplet temperature rises more gradually in the LES. The reasons for such differences can be attributed to different modeling of droplet dynamics in the CAS model. While droplets of different sizes can exist in the LES and URANS simulations, the CAS model assumes them to be monodisperse. Other factors include averaged modeling in CAS, which ignores the spatial distribution of droplets and hot ambient gas in the radial direction and the non-linear temperature dependency of the evaporation term. In the LES and URANS simulations, high temperatures exist in the outer regions and cold temperatures in the center. Droplets that move to the outer part evaporate quickly, while those in the center evaporate slowly. Such temperature distribution can affect the evaporation time, which may not be captured by the cross-sectional averaging.

### 4.6. Droplet Size Distribution

The CAS model was further extended in an attempt to obtain information on the droplet size distribution in the spray. Monodispersed droplet distribution was used for results in the previous sections by setting the PDF $P(\hat{d})$ to a delta function. As discussed before, the initial droplet size distribution at the nozzle exit must be known to use other PDFs. At high injection pressures and high ambient densities, the liquid fuel jet breaks into fine droplets very close to the nozzle, $\approx 10D_{noz}$, and therefore the secondary breakup processes may be negligible. For this reason, the KH-RT breakup model can be switched off, and only drag and evaporation govern the droplet dynamics, as shown by Davidovic et al. (2017) in their LES results. For comparability with these results, the breakup model was switched off in the CAS model and the URANS simulation for the case discussed in this section. In addition, $C_{vap}$ was set to unity in this case to reduce the evaporation rate.

Figure 12 shows the comparison of liquid and vapor penetration lengths for the LES, the URANS,
and the CAS model with Rosin-Rammler PDF as the initial droplet size distribution, which is obtained from the DNS of primary breakup of Spray A in Davidovic et al. (2017). The results of lognormal and gamma PDFs are not shown here, as they do not significantly differ from the Rosin-Rammler PDF. The liquid lengths from the LES and URANS simulations agree well with the measurements, whereas the CAS model underpredicts the liquid length. The lower liquid length in the CAS model is caused by the overestimation of the evaporation rate. The vapor penetration lengths from the LES and the CAS model match closely with that from the experiment. On the other hand, the URANS simulation largely underpredicts the vapor penetration for the reasons discussed before.

Within the liquid length, the droplet size distributions are compared in Figure 13 at two locations away from the nozzle. The shaded region indicates the variation within the steady-state period in the LES. Compared to the LES and URANS, the results of the CAS model with lognormal and gamma PDF represent the droplet size distribution at both locations reasonably. The Rosin-Rammler PDF is shifted to the right at 2 mm and is narrower than others, which leads to the conclusion that it may not be suitable for tracking the droplet size distribution in the reduced-order CAS model. On the other hand, the lognormal and gamma PDFs represent the droplet size distributions reasonably, and therefore may be used in the proposed approach.

The modeling approach for the polydisperse droplet distribution is presented here for demonstration. Although the results are encouraging, further investigations are needed on the discrepancies regarding the liquid length, which will be part of future work.

![Figure 13: Comparison of the droplet size distributions for case 1 from the URANS simulation and the CAS model at t = 1 ms on two locations away from the nozzle exit. The LES results are averaged in time (t = 1 ms to 2 ms), and the shaded region indicates the region of variation from minimum to maximum values.](image-url)
4.7. Computational Cost

All simulations were run on machines using the Intel Broadwell processor architecture. The 3D inert URANS of Spray A was run on 24 cores for \( \approx 1 \text{ h} \) for both delta and Rosin-Rammler initial droplet size distributions, resulting in a total of 24 CPUh. The CAS model with the delta PDF for droplet size distribution was run on a single core for \( \approx 45 \text{ s} \) (= 0.0125 CPUh) for the same case, which is a factor of 2000 compared to the URANS. For more complex droplet distributions, the computational cost of the CAS model increased to 0.125 CPUh for the Rosin-Rammler PDF, 0.8 CPUh for the gamma PDF, and 1.2 CPUh for the lognormal PDF. The LES, on the other hand, required 62 kCPUh for the blob injection (delta PDF) and 102 kCPUh for the Rosin-Rammler initial droplet size distribution. Thus, the improved CAS model is faster by up to 3 orders of magnitude compared to the URANS and 4-6 orders of magnitude compared to the LES and provides reasonable estimates for liquid and vapor lengths, mixing, as well as droplet size distribution for a wide range of conditions and potential novel bio-hybrid fuels.

5. Conclusions

In this paper, the original CAS model was evaluated with respect to experiments, LES, and URANS results to determine its capabilities to predict macroscopic spray characteristics such as liquid and vapor penetration, mean droplet diameter, and mixing. The original model performed well for different ambient densities, injection pressures, and nozzles; however, it failed to predict the trends in the spray characteristics for variation in ambient temperatures and different fuel properties for the given injector. Also, the model in its original form did not track the vapor mass fraction, which plays an important role in the evaporation model and provides information on local mixing with the ambient gas. In this work, the model was improved by replacing the Reitz-Diwakar breakup model with the state-of-the-art Kelvin-Helmholtz Rayleigh-Taylor model. An additional equation is solved for the fuel-vapor transport required for the evaporation model, and the non-equilibrium evaporation model proposed by Miller and Bellan was implemented. In addition, a phenomenological nozzle flow model was implemented to predict the nozzle exit velocity. The improved CAS model was able to reproduce the trends in global spray characteristics for different ambient temperatures as well as novel bio-hybrid fuel candidates.

The model was further extended to consider polydisperse sprays. A transport equation was derived for the mean droplet diameter, in addition to the existing equation for the squared droplet diameter, and the droplet size distribution was constructed from the presumed PDFs, namely Rosin-Rammler, lognormal, gamma distributions, fitted using the two moments of the droplet diameter. This approach was able to track the droplet size distribution along the axial coordinate of the spray, and lognormal and gamma distributions were found to be more suitable rather than the commonly used Rosin-Rammler
distribution.

The CAS model was developed to be a physics-based reduced-order model for various applications, which require parameter variation, sensitivity analysis, and real-time prediction, e.g., a rapid screening tool for a large number of novel bio-hybrid fuel candidates and model-based control of an engine. The 3D simulation methods are computationally expensive and hence not suitable for these applications. A posteriori computational cost analysis and comparison with 3D simulation methods showed that the improved CAS model with monodispersed droplets is faster by up to 3 orders of magnitude compared to the URANS and by up to 6 orders of magnitude compared to the LES. Modeling of the droplet size distribution increased the computational cost of the CAS model by a factor of 20-200 depending on the type of PDF used, with lognormal distribution as the most expensive and Rosin-Rammler as the least expensive distribution to compute.

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Appendix A. Original CAS Model

Appendix A.1. Governing Equations

The system of hyperbolic partial differential equations (PDEs) for the original CAS model of Wan (1997) are written as

\[ D_{\epsilon}(\bar{\rho}Y_{g}b^2) = \omega_{ent,g}b + \omega_{vap}b^2 \]  
\[ D_{\epsilon}(\bar{\rho}Y_{g}u_gb^2) = -\omega_{drag}b^2 + \omega_{vap}u_gb^2 \]  
\[ D_{l}(\bar{\rho}Y_tb^2) = -\omega_{vap}b^2 \]  
\[ D_{l}(\bar{\rho}Y_{l}u_lb^2) = \omega_{drag}b^2 - \omega_{vap}u_lb^2 \]  
\[ D_{l}(\bar{\rho}Y_{l}d^2b^2) = -\omega_{brd}b^2 - \frac{5}{3}\omega_{vap}d^2b^2 \]  
\[ D_{l}(\bar{\rho}Y_{l}T_db^2) = \omega_{heat}b^2 - \omega_{vap}T_db^2 \]
The two-phase mixture density is computed as
\[
\frac{1}{\bar{\rho}} = \frac{\dot{Y}_l}{\rho_l} + \frac{\dot{Y}_g}{\rho_g}.
\] (A.7)

Mass conservation requires \(\dot{Y}_l + \dot{Y}_g = 1\). The entrainment and the drag models were described in sections Section 2.2 and Section 2.3, respectively. Since the vapor and ambient gas are considered to be perfectly mixed and vapor mass fraction is not tracked explicitly, the gas mixture is denoted by subscript 'g'. The droplet breakup and the evaporation models are described briefly in the next sections.

**Appendix A.2. Droplet Breakup Model**

The Reitz and Diwakar (1986) (RD) wave breakup model was used for the secondary breakup, assuming that most breakups were of stripping-type (Reitz, 1987). The droplet breakup source term is computed as \(\dot{\omega}_{bre} = K_{bre}\dot{Y}_l\), where the breakup coefficient, \(K_{bre}\), is modeled as
\[
K_{bre} = \frac{2\hat{d}(\hat{d} - d_{st,\text{RD}})}{\tau_{b,\text{RD}}},
\] (A.8)
and the stable diameter is computed as
\[
d_{st,\text{RD}} = \frac{\sigma_l^2}{\rho_g \hat{u}^3_{rel} \mu_g},
\] (A.9)
where \(\sigma_l\) is the surface tension of the liquid. The stripping breakup time is computed as
\[
\tau_{b,\text{RD}} = C_b \frac{\hat{d}}{u_{rel}} \left(\frac{\rho_l}{\rho_g}\right)^{1/2},
\] (A.10)
where \(C_b\) is a model constant with a suggested value of 10 (Reitz and Diwakar, 1986).

**Appendix A.3. Evaporation and Droplet Heating Model**

Frössling (1938) correlations are used to model evaporation from the external droplet surface. The evaporation source term is computed as
\[
\dot{\omega}_{vap} = \frac{3K_{vap} \dot{\rho}\dot{Y}_l}{2\hat{d}^2},
\] (A.11)
where
\[
K_{vap} = 8\frac{\rho_g \Gamma_{v,g}}{\rho_l} \ln(1 + B_{M,d}) \text{Sh}_d.
\] (A.12)
\(\Gamma_{v,g}\) is the diffusion coefficient of fuel vapor (subscript 'v') in the surrounding gas mixture. The droplet mass transfer number is defined as
\[
B_{M,d} = \frac{Y_{v,s} - Y_{\infty,v}}{1 - Y_{v,s}},
\] (A.13)
where the vapor mass fraction on the droplet surface is modeled as

\[
Y_{v,s} = \frac{\chi_{eq,v,s}}{\chi_{eq,v,s} + (1 - \chi_{eq,v,s})WR},
\]

where \(WR = W_a/W_f\) is the ratio of the molecular weight of the ambient gas excluding vapor (subscript 'a') to the molecular weight of fuel (subscript 'f'). The subscript 's' denotes variables at the droplet surface. The equilibrium vapor mole fraction, \(\chi_{eq,v,s}\), at the droplet surface is computed as

\[
\chi_{eq,v,s} = \frac{p_v(T_d)}{P_g},
\]

where \(P_g\) is ambient gas pressure and \(p_v(T_d)\) the vapor pressure at the droplet temperature. For the cases considered here, \(Y_{\infty,v}\) is set according to the one-third rule (Hubbard et al., 1975) to \(Y_{\infty,v} = (\hat{Y}_v + 2Y_{v,s})/3\), where \(\hat{Y}_v\) is chosen to be zero, assuming the far-field value of the vapor mass fraction to be negligible. The droplet Sherwood number is computed as

\[
Sh_d = (2.0 + 0.6 Re_d^{1/2} Sc_g^{1/3}) \ln(1 + B_{M,d})/B_{M,d},
\]

with the gas-phase Schmidt number, \(Sc_g\), defined as

\[
Sc_g = \frac{\mu_g}{\rho_g \Gamma_{v,g}}.
\]

The heat transfer between the droplet and ambient gas mixture is modeled as

\[
Q_d = \frac{\lambda_g(T_{ref})(T_g - \hat{T}_d)}{\hat{d}}Nu_d,
\]

where \(\lambda_g(T_{ref})\) is the thermal conductivity of the local gas-phase mixture and \(\hat{d}\) the ambient gas temperature. The droplet Nusselt number is given by

\[
Nu_d = (2.0 + 0.6 Re_d^{1/2} Pr_g^{1/3}) \ln(1 + B_{M,d})/B_{M,d},
\]

and the gas-phase Prandtl number, \(Pr_g\), is defined as

\[
Pr_g = \frac{\mu_g(T_{ref})C_{p,g}(T_{ref})}{\lambda_g(T_{ref})}.
\]
$C_{p,g}(T_{\text{ref}})$ is the specific heat capacity of the gas-phase mixture at constant pressure. The gas-phase mixture properties and correlations are computed at the reference temperature, which is obtained by the one-third rule (Hubbard et al., 1975)

$$T_{\text{ref}} = \frac{T_g + 2T_d}{3}. \quad (A.22)$$

Since the boiling model is not used, the droplet temperature is kept bounded by an upper limit of saturation temperature at the given pressure. The ambient gas temperature is held constant throughout the domain at all times. The liquid properties such as density ($\rho_l$), surface tension ($\sigma_l$), and viscosity ($\mu_l$) are evaluated at a constant fuel temperature at the nozzle exit ($T_{l,o}$) and remain constant throughout the liquid phase. The gas-phase mixture properties, such as density ($\rho_g$), viscosity ($\mu_g$), thermal conductivity ($\lambda_g$), and specific heat capacity at constant pressure ($C_{p,g}$) are approximated by the corresponding properties of ambient gas only.

**Appendix A.4. Comparison with LES and URANS**

Figure A.14 shows the non-dimensional flow variables from the CAS model and the URANS simulation along the non-dimensional axial coordinate (defined in Table 3). The two-phase mixture density ($\rho^*$), mass fractions of the liquid ($Y^*_l$) and the ambient gas ($Y^*_g$), and velocity of the liquid phase ($u^*_l$) along the axial coordinate are shown in Figure A.14(a). Due to the Lagrangian description, these variables are not directly comparable with those from the LES and URANS simulations.

The gas-phase velocity is available in the URANS results for comparison, and its cross-sectional average is compared with the ambient gas velocity from the CAS model (see Figure A.14(b)). The LES results of the gas-phase velocity are not compared, as an ensemble averaging of several independent runs would be required, and these data are not available. High gas velocities are induced close to the nozzle in the CAS model, whereas velocities of similar magnitude occur in the URANS simulation at a farther location from the nozzle exit. The decay of the gas velocities in URANS is faster compared to that in the CAS model. These observations confirm the reasons discussed before for the underprediction of the vapor penetration in the URANS approach.

Figure A.14(c) shows the mean droplet diameters along the axis of the spray from the LES, URANS, and CAS models. The LES results are averaged in time during the steady-state phase. In the LES, the mean droplet diameter drops rapidly within a distance of $\approx 10D_{\text{noz}}$. In contrast, the mean droplet diameter in the URANS simulation decreases gradually over the liquid length. The CAS model shows trends similar to the URANS results, although the breakup models are quite different in the two simulation models, with combined KH-RT model in URANS and Reitz-Diwakar model in CAS.

The droplets in the LES and the URANS simulation heat up faster than those in the CAS model (see Figure A.14(d)). Also, the droplets in the CAS model survive up to much farther distances from
the nozzle. These discrepancies can be attributed to the monodispersed droplet assumption at each axial location in the CAS model, whereas droplets of different sizes can exist in the LES and URANS simulations. Also, the non-linear temperature dependency of the evaporation term is a possible second reason.

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