Spray combustion in engines

A few lecture hours and some pages of lecture notes are by far not sufficient to cover the broad subject of spray combustion in engines. As a matter of fact, dedicated journals and books exist on sprays. Therefore, the current lecture only serves as an introduction to the subject. Optimally, the lecture slides, text and references in this chapter should function as a “Quick Start Guide” to the vast literature on spray combustion in engines.

The scope of this chapter is as follows. After an introductory section, we will look at different phenomena in fuel sprays (e.g., with what speed and angle they move, how they break up, evaporate and ultimately combust). After that we discuss different classes of spray models, ranging from simple measurement-based correlations to full CFD models (without going into details on the latter). In the section 8 some (semi-)phenomenological models are treated in more detail, since these provide a good balance between simplicity and physical insight. Since the text was written for a post-graduate combustion course, the level of this chapter is slightly more advanced than the rest of the lecture notes. Therefore, from the models discussed, only the Sandia model belongs to the core part of the Fuels & Lubes course.

1 Introduction

From the previous chapter it is clear that fuel-air mixing is of utmost importance for the efficiency and emissions of the combustion process in engines. These days, fuel is very often introduced into the Internal Combustion Engine in the form of a spray. This holds true both for SI (spark ignition) and CI (compression ignition) engines; however, the spray regimes differ greatly.

In SI engines, the fuel is introduced together with the intake air, implying that injection takes place in a low temperature, low density environment. This has no great impact on the fuel-air mixing process: fuel volatility is generally high, and due to the early injection there is ample time for mixing. As a result, fuel and air in an SI engine are generally well premixed. Only few modern SI engines are using the concept of DI (direct injection), in which fuel is injected during the compression stroke. The result is then an overall lean mixture, which is however slightly rich near the spark plug, to facilitate spark ignition. This implies that some stratification is present, which is needed for optimal combustion in such (SIDI) engines.

Notwithstanding the importance of DI developments in SI engines, the current text (and lecture) will mostly focus on the direct injection process in DI diesel engines. Due to their generally higher compression ratio, combined with a broader use of turbochargers, the density at the moment of fuel injection is generally much higher. The same holds to some extent for temperature. As we will see, this has important implications for the fuel evaporation process in the spray.
In conventional diesel combustion, only a small portion of the fuel would burn in premixed mode. This holds for the portion of fuel that is injected first: it needs some time to vaporize, heat up and auto-ignite (i.e. the ignition delay, ID). After the ID, the resulting premixed region combusts quickly, resulting in the so-called “premixed peak” in the heat release, associated with the characteristic sound of a diesel engine (“diesel knock”).

The remainder of the fuel is then injected into this rich, premixed flame; as a result, most of it necessarily burns in a diffusion mode at the periphery of the spray. The process just sketched is nowadays understood fairly well; much of this understanding is often attributed to John Dec, who published his conceptual model on diesel combustion in 1997 [14]. The main summarizing picture from that reference is reproduced in Fig. 18.1. The picture shows a “mature” spray, which has reached its quasi-steady state (i.e. the upstream part of the spray stays more or less the same, whereas the head vortex is penetrating the combustion chamber further) after the injection transient. The latter is also addressed in Ref. [14], as well as in the lecture slides.

Recently, more and more emphasis is put on premixed combustion modes for diesel engines as well, as sketched in the previous chapter. In such combustion modes, ignition delay is generally larger, aiming at a separation of the injection and combustion events. Obviously, the resulting stratification of the fuel-air mixture (and, not unimportantly, of temperature!) prior to combustion is crucial to the efficiency and emissions reduction of these new combustion processes and, hence, of future engines.

In order to understand from basic principles how spray formation takes place, and how it results in a certain distribution of fuel/air ratio and temperature, this chapter deals with spray processes in a structured way. The description focuses on mixture formation before combustion, since a detailed understanding of the combustion process is necessarily beyond the scope of a one-hour lecture.

Hence, this chapter focuses on physical spray processes, including dynamics (spray penetration, breakup, air entrainment) and thermodynamics (evaporation). A smaller part of the chapter is devoted to the actual combustion phase. A better name for the chapter might therefore be “sprays in combustion engines” rather than “spray combustion in engines”.

**Figure 0.1:** Conceptual model of quasi-steady reacting diesel spray, adapted from Dec [14]
1.1 Life of a fuel spray

According to Wikipedia, a spray is “a dynamic collection of liquid drops and the entrained surrounding gas”. To my taste, this definition is a bit (too) broad, since it may also apply to, for instance, a rain cloud. Consulting some more sources on the web, it appears that – in spite of a very broad range of applications of sprays – there are common properties applying to all sprays.

Indeed a spray consists of droplets and entrained ambient gas. The existence of these droplets is the result of atomization, in which a liquid jet breaks up into droplets due to its high velocity. Typically, a spray issues from a small hole connected to a pressurized container. The liquid jet leaves the hole with very high velocity, giving rise to high levels of shear with the surrounding gas. In addition, a high speed liquid jet also exhibits intrinsic instabilities (some of these are briefly addressed later on), which present an additional cause for breakup.

In any case, the result is a fine mist of liquid droplets, which protrudes into the surrounding gas, entraining a significant portion of it. In this way, momentum is transferred from the droplets to the gas; as a result, the spray velocity decreases with distance from the nozzle hole. This process can be modeled with high accuracy using fairly simple models, as will be shown in section 8.

The tip of the spray travels into the gas in the form of a “head vortex”, which typically makes out 20 to 30% of the size of the full spray. The region behind the head vortex shows more or less straight edges (that is, on average; turbulent fluctuations are always present). Most air entrainment takes place along these edges.

The above description holds for all sprays, not only for those used in combustion systems. Typical for the latter (fuel sprays) is that the surrounding gas is hot. In addition, especially for DI diesel engines, the fuel injection pressure is typically very large (several thousand of bars), giving rise to extremely high velocities. Hence, the droplets resulting from atomization are extremely small, and quickly vaporize in the hot ambient gas.

Since combustion requires mixing on a molecular level, it only sets in after sufficient evaporation. Therefore, part of the observed ignition delay (ID) in engines is due to the evaporation process (the so-called “physical ignition delay”). The other part is due to the auto-ignition chemistry of the fuel (“chemical ignition delay”). It should be noted that these phases do not strictly follow each other, but take place simultaneously (although evaporation temperatures might be too low for significant auto-ignition chemistry to occur).

During the ignition delay period, the first portion of the spray has had time to premix with air. As pointed out before, this part then quickly combusts in a premixed rich flame. The trailing edge of the spray enters this hot premixed flame and alsoignites. The heat of combustion affects evaporation; likewise, the evaporation process will affect combustion (via temperature) due to evaporative cooling. After some time, a quasi-steady equilibrium distance sets in where the foot of the turbulent spray flame is located, the so-called flame lift-off length $H$ (the precise stabilization mechanism is still not fully understood, as will be addressed later)

All fuel entering this premixed flame will, at first, partly combust; the rich products travel further downstream, giving rise to soot formation. Ultimately, these rich products – and most of the soot – will oxidize in the turbulent diffusion flame surrounding the spray. This very hot diffusion flame front is the main location of NO formation in the engine. The resulting heat release causes the pressure to increase, which ultimately drives the engine. Unfortunately, part of the soot may not oxidize and is emitted with the exhaust gas.

When injection stops, the existing flame will consume the fuel remaining upstream. However, in cases where the flame lift-off is large, this part may become too lean to combust, in which case the end phase of injection is a source of unburnt hydrocarbons [50, 61, 47].
1.2 Measurement in fuel sprays

From the previous section it appears that a fuel spray has a fairly complex life “from the cradle to the grave” (end of combustion). Many processes take place, partly sequential, but mostly in parallel. Some of these processes are strictly physical in nature, others are (also) chemical. To understand these processes, how they interact, and how they ultimately translate into engine performance (power, efficiency) and emissions, requires a wide range of well-designed experiments.

Such experiments are complicated by the fact that an engine is not the easiest environment for measurements, to say the least. Pressures and temperatures are very high; the environment is highly reactive; and the geometry is constantly moving at a very high speed. To enable this combination of conditions, engines are necessarily constructed out of metal parts. Unfortunately, metals are not transparent. Consequently, most engine experiments are limited to measuring input-output relations (inputs: speed, intake pressure and temperature, fueling etc.; outputs: power, efficiency, emissions). Often, in-cylinder pressures are also monitored to enable some analysis of the in-cylinder processes. All these measurements are indirect and do not exhibit much detail of the spray process.

In order to capture the behavior of a combusting fuel spray, optical measurements are necessary. Introducing optical access to an engine is far from easy, although it can be done. Unfortunately, the engine will be different after such modification, depending on the extent of optical access provided: think of a changing piston head geometry (when replacing it with a – typically flat – window), and changing heat transfer rates for a Bowditch engine principle (where the piston head is put “on legs”). In spite of these drawbacks, visualization of spray combustion in real engines has been done by several groups (including the Nijmegen Molecular Physics group and the Eindhoven CT group). Some example results are shown in the lecture.

Measurements in optical engines are often not very quantitative. For a detailed understanding of fuel sprays and validation of spray models, measurements must be done in dedicated test setups. In such setups the engine environment is mimicked (providing high pressure and temperature), but with better optical access. Examples include shock tubes, rapid compression machines, modified (motored) engines, and so-called constant volume cells or “combustion bombs”. An overview – together with pro’s and con’s of each – is provided in a recent SAE paper by Baert et al. [7].

At Eindhoven University of Technology, spray research is mainly done in the Eindhoven High Pressure Cell (EHPC). Its operating principle is described at length in the paper just mentioned, and is briefly summarized here. A schematic picture is provided in Fig. 18.2. The EHPC is a constant volume cell, in which high pressure and temperature are created using pre-combustion. In this method, the EHPC is filled with a mixture of acetylene, nitrogen, oxygen and argon. The mixture is ignited by a spark and then explodes; when combustion is complete, the end gas cools down and then a fuel spray is injected with a chosen timing, based on the average temperature at that moment in the cell. The ambient gas density is constant over time, governed by the amount of mixture that is initially entered.

Depending on the initial gas composition, the injected fuel spray may or may not react. When pre-combustion is close to stoichiometric, no oxygen is left and the fuel spray will only vaporize. In the other case, when pre-combustion starts with a lean mixture, oxygen is left after it, and the fuel spray may still react. The properties of the pre-combustion end gas can be tuned to desired values (density, peak temperature, remaining oxygen fraction and specific heat) by adjusting the four intake masses (acetylene, oxygen, nitrogen, argon), as discussed in Ref. [7].

Since a constant volume cell has no moving parts, optical access can be granted easily through large windows (both quartz and sapphire windows are used; quartz has a better transparency for UV wavelengths, but sapphire can handle higher pressures). In Ref. [7], several examples of optical measurements are discussed. So far, mostly macroscopic spray phenomena (penetration, cone angle,
liquid length, flame lift-off) have been measured. This was mostly done using a combination of shadowgraphy, Schlieren, Mie scattering and natural luminosity measurements. Sample results are shown in the lecture. More generally, it must be noted that a variety of laser diagnostic techniques has contributed enormously to the understanding of sprays, both before [76] and during combustion [14]. For reasons of time and space, these methods will not further be discussed here.

![Cross-sectional overview of the Eindhoven High Pressure Cell and its main components](image)

**Figure 0.2:** Cross-sectional overview of the Eindhoven High Pressure Cell and its main components [7]

So far we did not address fuel injection equipment. For an excellent introduction, the reader is referred to Baumgarten [8]. For DI diesel engines, common rail systems are now most widely used. In such a system, multiple injectors are connected to a buffer vessel that is continuously kept on high pressure – in contrast to a conventional line pump, which works intermittently. The injector itself is mostly operated by electronically actuating the return valve, which causes the needle to rise. As a result, fuel is admitted to the nozzle holes (typically 100 to 200 µm in diameter).

Important for the spray formation process are mainly the mass flow and momentum flow out of an injector. To characterize its mass flow, the simplest way is collecting a number of injections in a container, weighing it, and dividing by the number of injections. In this way the integrated mass flow per injection is obtained. Comparing it with the theoretical value (see next section) provides a value of the discharge coefficient \( C_d \).

If time-resolved mass flow results are needed, the injector can be mounted into a so-called Zeuch chamber. This is a vessel that is pre-filled with the fuel of interest. Adding extra fuel gives rise to a strong pressure increase, caused by the incompressibility of the liquid fuel. By measuring the time resolved pressure, the mass flow during an injection can be obtained, which is important for engine calibration. More details on this method are provided by Seykens et al. [70].

To characterize the momentum flow from a nozzle, one should realize that force is equal to the change of momentum. Holding a plate perpendicularly in front of an injector nozzle hole, will cause the fuel spray to loose its momentum (since the fuel can only move perpendicularly to the plate). Connecting the plate to a force transducer, and thus measuring the associated force, gives a measure of the momentum flux from the nozzle hole. Although this measurement could in principle be done in a time-resolved fashion, usually only the average force is considered, and is then used to derive the momentum coefficient \( C_M \) (further addressed below), cf. Ref. [59].
2 Spray phenomenology

After the brief overview of the “life of a spray” in the preceding section, this section goes into more detail on the main processes involved in spray combustion. For each of these processes, the main parameters are introduced. By making the reader familiar with these concepts, it is hoped that the vast literature on spray combustion becomes better accessible. A number of references is provided as a starting point (but note that the cited literature is by no means intended to be complete).

2.1 Nozzle discharge

The flow through an injector nozzle hole is mainly governed by Bernouilli’s law. The theoretical exit velocity \( U_{th} \) and the pressure difference over the nozzle hole \( \Delta p \) are coupled according to

\[
U_{th} = \sqrt{\frac{2 \Delta p}{\rho_f}},
\]

where \( \rho_f \) is the (liquid) fuel density. The resulting (theoretical) mass flow rate equals \( \dot{m}_{th} = \rho_f U_{th} A_0 \), where \( A_0 = \pi d_0^2 / 4 \) is the geometrical nozzle cross-sectional area. Now Bernouilli’s law is only valid for an incompressible, frictionless flow, which is not fully true during nozzle discharge. However, the difference can be “repaired” by relatively simple corrections.

What actually happens in a nozzle hole is depicted in Fig. 18.3, taken from Payri et al. [58]. Fuel from the pressure reservoir rounds the inner corner, and strongly accelerates. Due to the resulting high velocities, the dynamic pressure strongly drops, causing local pressure to drop below the fuel’s saturation pressure. Consequently, the flow is cavitating. The bubbles formed are partly transported downstream with the fuel, changing the average density of the flow, as depicted on the right hand side of Fig 18.3. This can be interpreted as if the flow would have an effectively smaller outflow area for fuel of (liquid-only) density \( \rho_l \). The ratio of this effective area and the geometric area is \( C_a = A_{eff}/A_0 \), known as the area contraction coefficient.

The assumption of frictionless flow is also not fully correct: the exit velocity is smaller than the value obtained from Eq. (18.1). The difference is expressed in terms of the velocity contraction coefficient, \( C_v = U_{eff}/U_{th} \). Combining both effects, the real mass flow from the nozzle hole can be written as \( \dot{m} = \rho_f U_{eff} A_{eff} \). We can then define the ratio between the actual and theoretical mass flow; this is the discharge coefficient \( C_d \), defined by

\[
C_d = \frac{\dot{m}}{\dot{m}_{th}} = \frac{U_{eff}}{U_{th}} \cdot \frac{A_{eff}}{A_0} = C_v \cdot C_a.
\]

Following similar arguments, we can also compare the real momentum flux with the theoretical one. The latter obviously is \( M_{th} = \rho_f U_{th}^2 A_0 \); similarly, the effective momentum flux is \( M = \rho_f U_{eff}^2 A_{eff} \). Comparing the two in a ratio provides the momentum coefficient \( C_M \), given by

\[
C_M = \frac{M}{M_{th}} = \left( \frac{U_{eff}}{U_{th}} \right)^2 \cdot \frac{A_{eff}}{A_0} = C_v^2 \cdot C_a = C_d \cdot C_v.
\]

Effectively we have chosen \( A_{eff} \) and \( U_{eff} \) such, that the resulting mass and momentum flows follow the idealized expressions above. As indicated in the previous section, both \( C_d \) and \( C_M \) can be obtained from fairly straightforward experiments. Combining them, using the preceding two equations, enables one to obtain the velocity and area contraction coefficients as well, as detailed for instance in Ref. [58]. These values are needed in most of the phenomenological models to be discussed in section 8.
Figure 0.3: Left: schematic overview of internal nozzle flow with flow separation. Right: definition of effective velocity and surface area. Source: Payri et al. [58]

Unfortunately, the values of the “constants” thus obtained are not really constant with conditions. They are found to depend on the amount of cavitation that occurs in the nozzle hole [58]. Cavitation occurs if the pressure in point c in Fig. 18.3 drops below the fuel’s saturated vapor pressure \( p_v \). If the flow accelerates even further, the thermodynamic equilibrium that sets in will keep the local pressure equal to \( p_v \). Using Bernoulli from point i to c, continuity in c and the definition of \( C_d \), it can be shown – cf. Desantes et al. [20] – that the discharge coefficient then equals

\[
C_d = C^c \sqrt{\frac{p_i - p_v}{p_i - p_b}} \equiv C^c \sqrt{K}.
\] (4)

In this equation the cavitation number \( K \) is introduced, which is equal to 1 for strongly cavitating flows. The larger \( K \) gets, the less cavitation occurs, until a value \( K = K_{\text{crit}} \) is reached where cavitation disappears (typically \( K_{\text{crit}} \approx 1.1 \)). The constant \( C^c = A_c/A_0 \) is the ratio of the vena contracta surface area to that of the nozzle hole, and is assumed to be constant for a given nozzle.

Coming from the other limit (i.e. initially non-cavitating flow at moderate values of \( p_i \)), \( K \) initially is a (weak) function of the Reynolds number. When it gets below \( K_{\text{crit}} \), thus when cavitation sets in, an interesting combination of phenomena happens, see Fig. 18.4. The momentum coefficient \( C_M \) is hardly affected by cavitation and remains constant. The mass flow, however, is choked at the critical value; a further decrease of \( K \) (for instance by lowering \( p_b \)) will not further increase \( \dot{m}_f \). Accordingly, \( C_d \) goes down with decreasing \( K \). This can only happen – see Eqs. (18.2) and (18.3) – if \( C_v \) increases, whereas \( C_o \) decreases more strongly. Physically, this is attributed to the effect of cavitation as follows: the bubbles in the flow decrease the amount of wall shear, enabling the velocity to increase, but at the same time decreasing the effective area of the liquid phase [58].
In diesel applications, back pressures are typically between 2 and 7 MPa; common rail pressures are typically around 200 MPa. As a result, practical values of $K$ are around 1.02, so very close to 1 and in the sensitive area of Fig. 18.4. In principle, the above dependence of nozzle coefficients on conditions should be taken into account when using experimentally measured constants in applications with different $K$; still, the variation of $K$ is limited in an absolute sense, so as a first approximation using constant values is not that bad.

Apart from pressure conditions, discharge coefficients depend on details of nozzle hole geometry. Such effects – on spray dynamics as well as on engine performance – have been extensively studied by the Valencia group, see for instance Refs. [57, 58, 59, 20]. Interestingly, in some of these works the experimental findings are combined with the inspection of polymer moulds of the nozzle holes. As an example, it was found that convergent nozzle holes show almost no tendency for cavitation, which is attributed to the fact that the entrance corner of such nozzles is less sharp.

In summary, we have seen in this section that nozzle discharge is governed by Bernouilli’s law; deviations from it are partly attributable to the vena contracta effect, typically in combination with cavitation. The resulting correction factors for mass and momentum flow and for velocity and surface area have been discussed. In first approximation, these correction factors are constant for a given nozzle when conditions do not vary too widely. However, they do depend on individual nozzle hole geometry.

Finally, a remark is in place about the injection pressure $p_i$ used above. It was so far assumed to be constant; in practice, the internal flow dynamics of an injector (and the upstream common rail system) causes significant variation in $p_i$ (typically ±5%) due to liquid phase compressibility effects. As a result, the mass flow from the injector also varies during injection. For the concepts discussed here this constitutes no big problem; for accurate engine operation, however, it needs to be taken in to account. For this reason, quite some work is often done to model the hydrodynamic behavior of the injection system (including common rail). Dedicated software is available that allows such modeling, for instance AMESIM (see, for example, Ref. [70]) and HYDSIM (cf. [65]).
2.2 Breakup, droplet size and cone angle

From the previous section it is clear that the fuel, emanating from a nozzle hole in a modern diesel injector, exits with a very high velocity and generally contains cavitation bubbles. Both observations give rise to a process named breakup. The latter is subdivided into primary and secondary breakup. During primary breakup, the remaining part of the intact liquid core is torn apart into ligaments and (relatively large) droplets. Secondary breakup is the process by which these droplets are broken up into smaller ones. In a review paper of Smallwood and Guld er [76], ample evidence is provided that breakup in contemporary diesel sprays has fully taken place after only a few nozzle diameters.

Primary breakup is the consequence of three effects: imploding cavitation bubbles (since the pressure in the cylinder \( p_b \) will normally be larger than the saturated vapor pressure \( p_{v} \)); turbulence within the liquid phase; and – to a lesser extent, cf. Refs. [76, 8] – aerodynamic forces acting on the liquid surface [77]. The balance between these mechanisms is governed by the Reynolds number \( Re = \rho_f U_0 d/\mu_f \) (ratio of inertia to viscous drag) and the Weber number \( We = \rho_f U_0^2 d/\sigma_f \) (ratio of inertial to surface forces).

Ohnesorge [53] showed that a convenient classification of breakup regimes could be obtained in terms of \( Re \) and the Ohnesorge number \( Oh = \sqrt{We/Re} = \mu_f/\sqrt{\rho_f \sigma_f d} \) (ratio between viscous drag and surface tension). Since both \( Re \) and \( Oh \) are formulated in terms of liquid properties only (whereas the density of the ambient gas definitely affects breakup), Reitz and Bracco latter added the density ratio \( \rho_g/\rho_l \) as a third parameter [67].

Depending on these numbers, different regimes of primary breakup exist. For very high \( Re \) and \( We \) (i.e. high velocity, resulting in a dominant role for inertial forces), the main breakup regime is atomization, characterized by a fast and vigorous breakup into small droplets, a conical shape of the liquid core at the nozzle and a diverging spray angle. The precise mechanisms behind it are still not fully revealed, in view of the difficulty to experimentally access the near-nozzle region.

Still, some detailed models of primary breakup are available. For the atomization regime, a model describing the dominant effects of turbulence and cavitation exists [77, 8], describing the redistribution of the sum of turbulent kinetic energy and cavitation implosion energy, into vapor-liquid surface energy and a velocity component perpendicular to the spray axis. The latter is directly responsible for the characteristic conical shape of atomizing sprays (further addressed below).

During secondary breakup, fuel droplets further disintegrate. This process is primarily governed by the Weber number, since it results from the trade-off between inertial forces (trying to tear the droplet apart) and surface tension (keeping it together). Again different regimes exist; for more details the reader is referred to literature, for example Refs. [77, 8]. The same holds for the description of interaction of droplets with each other and (possibly) with the cylinder wall.

In terms of spray combustion, the two most important results of the breakup process are the resulting spray cone angle and the droplet size distribution. From the above, it will be clear that a detailed prediction of these parameters from the basic underlying processes is by far not easy. Although commercial CFD packages often have breakup submodels on board, these contain a huge number of tunable parameters, each with their own uncertainty. What is more, as discussed in the next section, these parameters are often tuned in CFD computations in order to “compensate” grid dependencies.

As a result, predicted results of both cone angle and droplet size are often not very reliable. In addition, we have seen in the previous section that, for instance, the cavitation process is significantly affected by details of the nozzle geometry. In other words, the precise balance and magnitude of individual breakup processes will depend on details of each individual nozzle hole. De facto this will also hold for cone angles and droplet size distributions.
In view of these difficulties, many experimental efforts have been done to provide correlations for cone angles and droplet size distributions in terms of other parameters (fuel and ambient properties and injection parameters). Depending on what has been varied, these correlations capture more or fewer effects or parameter dependencies. Examples are provided below, first for droplet size and then for spray cone angles.

Droplet diameters in sprays are most conveniently expressed in terms of Sauter Mean Diameter (SMD). It defines an “average” droplet diameter in terms of having the right surface to volume ratio, which is of importance in droplet evaporation. In other words, SMD is proportional to the total volume of all droplets divided by their total surface area: from simple geometry, \( \text{SMD} = \frac{6V}{A} \).

Hiroyasu et al. [32] have correlated many measurements of SMD for relevant diesel conditions as a function of injection parameters (nozzle diameter and injection velocity), liquid surface tension and viscosity and density of both ambient gas and liquid. They provide two different correlations for SMD, one for incomplete and one for complete atomization. The final result of their work is

\[
\text{SMD} = \max \left[ 4.12 \text{Re}^{0.12} \text{We}^{-0.75} \left( \frac{\mu_f}{\mu_a} \right)^{0.54} \left( \frac{\rho_f}{\rho_a} \right)^{0.18}, 0.38 \text{Re}^{0.25} \text{We}^{-0.32} \left( \frac{\mu_f}{\mu_a} \right)^{0.37} \left( \frac{\rho_f}{\rho_a} \right)^{-0.47} \right],
\]

which is valid over a very large range of parameters. Among these are injection pressures up to 90 MPa and nozzle diameters down to 0.2 mm, which is just not sufficient to cover modern diesel conditions. The first entry between square brackets pertains to incomplete sprays (associated with less violent injection conditions). The second entry describes completely atomizing sprays, which will generally be more relevant for our purposes.

In the original paper [32] the notation of kinematic and dynamic viscosity is not used consequently, which gives rise to confusion (on a side note, the Hiroyasu group are not very strict in providing proper nomenclature). Still, a detailed study of the manipulations in the paper has shown that the above equation is correct if \( \mu \) is interpreted as dynamic viscosity. In their final Fig. 18, a very good correlation quality of the above equation with their data is shown.

More importantly, that same figure shows that the great majority of values of SMD/\( d_0 \) is between 0.1 and 0.3. Closer investigation of Eq. (18.5), writing the definitions of \( \text{Re} \) and \( \text{We} \) in full, shows that SMD/\( d_0 \) scales with \( d_0^{-0.07} \) – so hardly depends on \( d_0 \) – and with \( U^{-0.39} \). The higher the exit velocity, the smaller the normalized value of SMD gets. From this we can conclude that even smaller values of SMD/\( d_0 \) will be obtained for modern diesel conditions (higher injection pressures and smaller nozzles).

Therefore, as an indication, SMD \( \leq 0.1 d_0 \) can be used. This is confirmed by measurements of Desantes et al. [15], who use nozzles holes of 0.23 mm and find typical SMD values between 15 and 25 \( \mu \)m. They also compare the predictions of Ref. [32] to their experimental findings and conclude that they fit very well, in spite of the fact that the injection conditions are beyond the original fit range.

Although other SMD correlations are available in literature, Eq. (18.5) still is the most popular, since it is based on a very large quantity of measurements. Examples of its use can be found in Refs. [82, 40]. In these papers, the assumption is made that all droplets have the same diameter SMD. Yet, in principle, the size distribution is also important in spray modeling. In some other cases, a log-normal distribution having the same SMD is therefore assumed. However, droplet sizes resulting from (primary and secondary) breakup in modern diesel engines are so small that they evaporate almost instantly, depending mainly on the rate of air entrainment. This so-called mixing limited vaporization will be discussed later. Hence, droplet size distributions might be less important after all, and are therefore not further discussed here.
The spray cone angle $\theta$ plays an essential role in the models to be discussed in section 8, since it largely determines the air entrainment rate. The latter in turn determines both the rate of evaporation in the spray and the resulting equivalence ratio field throughout the spray. Therefore, the cone angle is of key importance for the (efficiency and emissions of the) combustion process.

A great variety of correlations for $\theta$ exist. An often used one is from Hiroyasu and Arai [31]:

$$\theta^{\circ} = 83.5\left(\frac{L}{d_0}\right)^{-0.22}\left(\frac{d_0}{d_s}\right)^{0.15}\left(\frac{\rho_a}{\rho_f}\right)^{0.26},$$  \hspace{1cm} (6)

where $L$ the nozzle hole length and $d_s$ the sack diameter. Physically, if $L/D$ is small, cavitation bubbles do not collapse inside the nozzle but are convected outwards; by collapsing there, they increase the cone angle. An older correlation by Hiroyasu and coworkers [30] is

$$\theta = 0.05\left(\frac{d^2\rho a}{\mu_a^2}\right)^{0.25}. \hspace{1cm} (7)$$

A correlation recommended by Heywood [27] but originating from Reitz and Bracco [66] reads

$$\tan(\theta/2) = \frac{4\pi}{3.0 + 0.28(L/d_0)}\left(\frac{\rho_a}{\rho_f}\right)^{0.5}\frac{\sqrt{3}}{6}. \hspace{1cm} (8)$$

Naber and Siebers [52] provide the following cone angle correlation for vaporizing sprays:

$$\tan(\theta/2) = 0.27\left(\frac{\rho_a}{\rho_f}\right)^{0.19} - 0.0043\left(\frac{\rho_f}{\rho_a}\right)^{0.5}. \hspace{1cm} (9)$$

Not all of the above correlations are in terms of the same parameters; depending on what specific authors have varied, they cast their fit into a specific form. Another (seemingly trivial) point of concern is that the cone angle $\theta$ and the half angle ($\theta/2$) are often interchanged, leading to factors of 2 appearing and disappearing again in different citations. The message is that one should always be very careful using correlations from others; preferably these should be checked against in-house data. A second, but equally important, argument to use in-house data is the effect of individual nozzle geometry, discussed before.

The definition of the correlation parameters is also very important. As an example, correlation Eq. (18.7) was measured in cold gases, and results were correlated as a function of (cold) gas viscosity. If the fuel spray enters a hot cylinder, should viscosity then be determined at in-cylinder conditions or at standard conditions? The answer can only be provided by comparison with hot measurements in which again viscosity is varied – however, such measurements are often not available.

In spite of the above remarks, we can conclude that the spray cone angle in all cases depends on the density ratio between ambient gas and liquid fuel. A second important parameter is the aspect ratio $L/d_0$ of the nozzle hole, which is however not present in all correlations (practical values are fairly constant, around 5; therefore this is often not systematically varied).

Dependence of cone angles on the kind of ambient gas has been investigated by Di Stasio and Allocca [23]. They conclude that the cone angle is mainly governed by the density ratio, and to a lesser extent by gas viscosity (however, their result shows that $\theta$ linearly increases with viscosity, in contrast to what Eq. (18.7) suggests). Yet, since the composition of the ambient gas in diesel engines is always very close to air, this effect is not too important for our present purposes.

In summary, use of the above correlations might provide a good estimate of cone angles, but their absolute accuracy should not be overestimated.
2.3 Penetration

As briefly discussed in the introduction (and in a great many papers, cf. [52, 79, 6, 23, 42, 21, 54, 47] to name just a few), spray penetration can be characterized as follows. After leaving the nozzle, the spray quickly atomizes and the resulting mixture of (very small, continuously evaporating) droplets and entrained air protrudes the combustion chamber. The head of the spray continuously meets stagnant air, and as a result develops a “head vortex”. A typical example is shown in Fig. 18.5, together with the definitions of penetration length $S$ and cone angle $\theta$.

Behind the head vortex, spray edges are – on average – relatively straight, with the exception of intermittently developing smaller side vortices. This region is commonly denoted as “quasi-steady”: although it grows in length (following behind the head vortex), processes in that region are – again on average, i.e. apart from turbulent variations – invariant with time during the steady phase of fuel injection. The latter typically occurs for Common Rail injectors, which show an almost top-hat injection profile, cf. [70, 21]. Since the fuel decelerates in the head vortex, the central velocity in the quasi-steady region is higher than that of the spray tip [21].

![Figure 0.5: Picture of penetrating fuel spray (EHPC data) showing penetration, cone angle and liquid length](image)

Most important for the diesel process is the speed of spray penetration. Two regimes can be distinguished. Initially, the spray leaves the nozzle hole with a “Bernoulli-like” velocity; there has not yet been significant air entrainment. As a result, the velocity is initially constant and $S(t) \propto t$. At later stages, further from the nozzle, we have a constant cone angle, which means that there is a constant rate of air entrainment (see section 8). As a result, the overall mass contained in the spray in each slice is proportional to its position $x$. Due to conservation of momentum (total mass times velocity = constant), we have $xdx/dt = \text{const.}$, leading to $x \propto t^{1/2}$. In other words, further away from the nozzle, spray penetration goes with the square root of time due to momentum conservation.

In between these limiting cases, there is a transition from the “linear” (dominated by liquid) to the “square root” (dominated by entrained gas) regime. This transition has been quantified differently by different authors, as will be discussed later. The experimentally observed transition time is usually on the order of 0.5 ms. This is comparable with typical opening times of a diesel injector; consequently, it is not fully clear whether the observed transition is due to the above mechanism or to finite injector response, as Desantes et al. argue [22]. In the latter case, it is not fully clear why the initial $S(t)$ transient would be exactly linear in time.

In many publications, the spray tip penetration $S(t)$ is fitted as a power of time. Logically, in view of the above, exponent values are usually found slightly above 0.5, cf. [79, 22, 43].
2.4 Evaporation

The above considerations on spray penetration hold for the fuel in general, independent of its phase. That is, for non-vaporizing (liquid) sprays the same overall behavior is observed as for vaporizing sprays (although the method of observation differs; liquid sprays can be observed using shadowgraphy, whereas the vapor phase can only be visualized using Schlieren methods). The reason is that spray penetration is purely determined by dynamics (masses and velocities of fuel and air).

In case of a vaporizing spray, the vapor phase shows the same tip penetration characteristics from the previous section. The liquid phase initially travels together with the vapor phase [61], but after some distance it “stops”; that is, no liquid is observed anymore. This distance remains quasi-steady (again apart from turbulent fluctuations) during the steady fuel injection phase, and is commonly denoted as “liquid length” $L$ [74, 79, 54].

The observation of such a quasi-steady liquid length is due to continuous air entrainment. At a certain distance from the nozzle, there is a balance between the amount of heat entrained by the hot air, and the amount of heat required for full vaporization. Quantification of this balance will be discussed in section 8.

Much attention has been devoted to measurement and interpretation of the quasi-steady liquid length in diesel fuel sprays, since it largely determines possible liquid fuel impingement on cylinder walls (known as “wall-wetting”) [11]. However, looking into more detail, also a “liquid width” exists: at a certain distance from the nozzle, liquid is only present up to a certain radial position as well. This establishes itself in the liquid phase showing a smaller apparent cone angle than the vapor phase (cf. [74, 28, 43], also visible in Fig. 18.5. In phenomenological models that include the radial spray direction, this behavior is accounted for, see section 8.4. It is important if one aims to make detailed predictions of the overall equivalence ratio and temperature field in the vicinity of the spray.

Conceptually, the quasi-steady liquid penetration is ultimately determined by droplet evaporation. However, there are many cases in which only the end stage of droplet evaporation is important, since evaporation transients are typically much faster than the timescale of mixing in modern diesel sprays (again related to the very small droplet sizes after breakup). This will be explained below.

Droplet evaporation has been discussed by many authors. Didactically, the book of Turns [78] can be recommended (although he causes some confusion by using the gas mixture specific heat $c_{pg}$ where it should be fuel vapor specific heat $c_{pf}^v$ in Eqs. (18.10)-(18.11) below). The latter point is also noticed in an excellent review paper by Sazhin [69], who discusses many aspects of droplet evaporation in great detail. In his conclusions, Sazhin states that the model by Abramzon and Sirignano [4] is still widely used since it combines accuracy and computer efficiency. A good example of its use is the paper by Hohmann and Renz [36], which is of very good quality and resolves some small shortcomings and provides some updates to correlations used in Ref. [4]. Below, the equations governing droplet evaporation are summarized, as combined from the references just discussed. Details of their derivation are not provided, but can be obtained/discussed on request.

The mass flow $\dot{m}$ from an evaporating droplet of radius $r_s$ can be obtained from both mass diffusion and from energy conservation. Both routes result in different expressions, which are however coupled via the temperature $T_s$ at the droplet surface [78]. These expressions are:

\[
\dot{m} = 2\pi\rho_g D_{fa} r_s \left[ 2 + \frac{Sh_0(Re) - 2}{F(B_M)} \right] \ln(1 + B_M) \tag{10}
\]

\[
\dot{m} = 2\pi \frac{k_s}{c_{pf}^v} r_s \left[ 2 + \frac{Nu_0(Re) - 2}{F(B_T)} \right] \ln(1 + B_T), \tag{11}
\]

where $\rho_g$ is the gas phase density, $D_{fa}$ is the binary diffusion coefficient of fuel in the ambient gas and
The thermal conductivity coefficient of the vapor phase. The universal function $F$ is defined by [4]

$$F(B) = \frac{(1 + B)^{0.7}}{B} \ln(1 + B). \quad (12)$$

The mass and heat transfer numbers $B_M$ and $B_T$ are given by

$$B_M = \frac{Y_{f,s} - Y_{f,\infty}}{1 - Y_{f,s}} \quad (13)$$

$$B_T = \frac{c_g p_f (T_\infty - T_s)}{\Delta H_{vap,f}(T_s) + Q_{i\to l}/\dot{m}}. \quad (14)$$

The saturated fuel vapor fraction $Y_{f,s}$ can be obtained from Eq. (18.20) below. Conditions far from the droplet are denoted by subscript $\infty$.

The internal droplet heating $Q_{i\to l}$ is often neglected, in which case the heat flux to the droplet is just balancing the mass flux from it times the heat of vaporization $\Delta H_{vap}$. For steady far field conditions, the droplet surface temperature $T_s$ is then steady (an effect that is for instance used in certain types of household hygrometers). This so-called “wet-bulb approximation” is often reasonably accurate.

More advanced approaches to account for instationary droplet heating are discussed by Sazhin [69]. Amongst those, the effective conductivity model is recommended [3]. This model accounts for the increased heat transfer due to internal circulation within the droplet, by using an effectively higher liquid heat conductivity coefficient. Especially when combined with the “parabolic model” [24], the effect of instationary droplet heating can be taken into account in an efficient and elegant way.

The Sherwood and Nusselt numbers above, $Sh_0$ and $Nu_0$, are given by

$$Sh_0(Re) = Nu_0(Re) = 1 + (1 + ReSc)^{1/3} f(Re), \quad (15)$$

where

$$f(Re) = 1, \quad Re \leq 1; \quad \text{and} \quad Re^{0.077}, \quad 1 < Re \leq 400. \quad (16)$$

The Reynolds number $Re$ is evaluated for the relative velocity between droplet $u_d$ and gas $u_\infty$, so

$$Re = 2 r_s \rho_\infty |u_\infty - u_d|/\mu_g,$$  

where $\mu_g$ is the gas phase dynamic viscosity. When the present evaporation model is embedded in a spray model, the relative velocity is evaluated using the following equation describing the droplet dynamics [36]:

$$\frac{du_d}{dt} \left(1 - 0.5 \frac{\rho_\infty}{\rho_f}\right) = \frac{3C_D}{8r_s} \left(\frac{\rho_\infty}{\rho_f}\right) (u_\infty - u_d)^2 \quad (17)$$

This equation can be derived from the definition of the drag coefficient $C_D$, in combination with elementary expressions for the mass and frontal surface area of the droplet. In Ref. [4] this equation is a factor of 4 in error, which was repaired later in Ref. [3]. The term in brackets on the left hand side of Eq. (18.17) accounts for the extra inertia that a droplet experiences in a gas [68]. Finally, the drag coefficient $C_D$ can be evaluated from

$$C_D = \frac{24}{Re} (1 + 0.15 Re^{0.687}) (1 + B_T)^{-0.2}. \quad (18)$$

Wherever fluid properties of the gas mixture are needed in the above equations, these are to be evaluated at temperature $\bar{T} = \frac{2}{3} T_s + \frac{1}{3} T_\infty$. When composition is needed, a value $\bar{Y} = \frac{2}{3} Y_s + \frac{1}{3} Y_\infty$ is recommended. This is known as “Hubbard’s rule” [37].
Obviously, quantitative results of the above model depend on the initial droplet size. For the latter, sometimes correlations are used (see for example Ref. [40]); others use experimental data [46] or compute it from detailed breakup models, cf. [35, 36, 38].

In spite of the complexity of the above equations, the results are easily summarized qualitatively. Initially, when a droplet enters a hot, unsaturated environment, it will evaporate according to the so-called “d^2 law”, i.e. the square of its diameter will decrease linearly with time. During this phase, the droplet is in quasi-steady equilibrium with its surroundings: although its diameter is decreasing, its temperature and evaporative mass flux are constant in time.

However, during this process, fuel vapor is continuously transferred to the droplet environment. Since droplets are close within a spray, each of them only has limited space available and the result is that its environment quickly saturates. Consequently, the rate of evaporation decreases and the droplet’s size reaches an equilibrium value. This is qualitatively sketched in Fig. 18.6.

Figure 0.6: Droplet-in-a-box, evaporating down to the saturation limit determined by mixing

In conventional diesel spray modeling, the above process is usually modeled in full detail, which gives rise to numerical issues (as discussed in the next section). However, as it appears, conditions in modern diesel sprays are often such, that the time scale of droplet evaporation is much smaller than that of mixing [76, 52, 16]. In Fig. 18.6, this implies that the droplet diameter very quickly “falls down” to the equilibrium level indicated by the dashed lines. Further evaporation then only occurs if that equilibrium level shifts – it only does so due to additional air entrainment. For this reason, this type of evaporation is denoted as mixing-limited vaporization, in which local transport processes around the droplet are “unimportant”, in the sense that they are fast enough in order not to be limiting.

In the latter case, only the description of the limiting case is needed; this situation corresponds to thermodynamic equilibrium between the droplet and its surroundings. It can be demonstrated that this equilibrium state only depends on the properties and thermodynamic conditions of fuel and air, and on the masses available of both (i.e. it does not depend on details of the droplet distribution). This is illustrated in Fig. 18.7, which shows equilibrium vaporization in a system at constant pressure $p_a$ (didactically corresponding to the in-cylinder ambient pressure), starting from masses $m_f$ and $m_a$, each with their own initial temperature.
When \( m_a \) in Fig. 18.7 increases, there will be a certain ratio \( m_a/m_f \) for which the ambient air carries just enough energy to evaporate all the (initially liquid) fuel. For that situation, \( m_{\text{evap}} = m_f \).

The end state is then, in view of the constant pressure, characterized by an enthalpy balance in which the enthalpy gain of the fuel is equal to the enthalpy loss of the ambient gas:

\[
m_f [h_f^g(T_s) - h_f^l(T_f)] = m_a [h_a(T_a) - h_a(T_s)].
\]

(19)

At the same time, the composition of the resulting mixture is characterized by saturation of the fuel vapor at temperature \( T_s \) (and, strictly speaking, at pressure \( p_a \) although the latter effect is generally small [44]):

\[
\frac{m_f}{m_a + m_f} = \frac{M_f \cdot p_{f, \text{sat}}^a(T_s)}{M_a \cdot [p_a - p_{f, \text{sat}}^a(T_s)] + M_f \cdot p_{f, \text{sat}}^a(T_s)} \equiv Y_{f, \text{sat}}^a(T_s).
\]

(20)

The preceding two equations form a coupled system for the saturation temperature \( T_s \) and saturated fuel mass fraction \( Y_{f, \text{sat}}^a \). This will return in different forms in the mixing-limited phenomenological models to be discussed later. Importantly, this system of equations does not contain any information on the spray geometry; it is purely a thermodynamic equilibrium. Spray details come in via the local mixing rate \( m_a/m_f \), which is, as argued before, only governed by dynamic processes (fuel mass and momentum conservation).

Before turning to a more quantitative description of fuel penetration and vaporization, we will now briefly discuss combustion in sprays, in order to complete our description of different phenomena involved in a combusting diesel spray.

### 2.5 Combustion

Only a few decades ago, the picture of combustion in diesel sprays was dramatically different from current understanding. As summarized by Dec [14], there was considerable debate whether fuel droplets would burn individually (with a small flame around each of them) or in groups. For brevity’s sake this discussion will not be repeated here.

Based on a number of laser diagnostic studies, available roughly since the 1980’s, the current understanding is that the liquid droplets have already fully evaporated in regions where flames exist, as pointed out earlier in this chapter. This holds both for the rich premixed flame upstream of the spray and for the diffusion flame surrounding it. For this reason, the main thing to understand is how atomization and droplet evaporation affect the resulting \((\phi, T)\) – temperature and equivalence ratio – fields in the spray. Accordingly, recent spray models often only deal with the liquid phase to derive effective source terms of fuel vapor, momentum and energy. This will be more extensively discussed in section 7.
The most important phenomena in spray combustion are auto-ignition, flame stabilization (and the associated lift-off length) and formation of emissions (mainly NO\textsubscript{x} and soot/PM, particulate matter). Auto-ignition takes place when the first part of the injected fuel has mixed with sufficient air to reach the right (\(\phi, T\)) conditions. This process has been dealt with in the previous chapter and will not be addressed in any more detail here (although its importance can hardly be overestimated!).

During the quasi-stationary phase of spray combustion, the rich premixed flame, initially resulting from auto-ignition, is stabilized at a certain distance \(H\) from the nozzle (again quasi-stationary, i.e. high-frequently varying due to turbulence). This distance, known as the flame lift-off length (FLoL) has been extensively measured and correlated as a function of temperature, density, nozzle diameter and injection pressure by the Sandia group [72]. From their results, Pickett \textit{et al.} derive the following correlation for normal diesel fuel [64]:

\[
H = 7.04 \cdot 10^8 T_a^{-3.74} \rho_a^{-0.85} d_0^{0.34} U_0^{1} Z_m^{-1},
\]

where \(H\) is in [mm], \(d_0\) in \(\mu\text{m}\) and other quantities have their normal SI units. In additional papers, the effects of ambient oxygen concentration [73] and fuel oxygen [49] on \(H\) were investigated.

For measurements of \(H\), chemiluminescence of OH radicals is used, a method that is critically evaluated in Ref. [71]. It must be noted that observations of lift-off lengths are sometimes reported in terms of natural soot luminosity of the flame, also known as the "soot lift-off length" (SLoL). Since soot particles need finite time to form and grow before they significantly radiate, SLoL is always larger than FLoL and thus provides an overestimate of the real flame lift-off length based on OH as a flame front marker.

Higgins and Siebers in Ref. [71] also compare their values of \(H\) to previously measured values of the liquid length \(L\). They conclude that either of the two can be larger than the other, depending on prevailing conditions, see Fig. 18.8 for an illustration. Increasing ambient density and temperature tend to make \(H\) smaller than \(L\). On the other hand, higher injection pressure, smaller nozzle holes and increasing EGR levels have the reverse effect. The latter three are the main trends in modern diesel engines – hence, it seems that the trend is towards \(H > L\).

\[\text{Figure 0.8.} \text{ Flame lift-off } H \text{ versus liquid length } L. \text{ Left: } H < L; T_a = 1100 \text{ K}, \rho_a = 23 \text{ kg/m}^3, p_i = 40 \text{ MPa and } d_0 = 250 \mu\text{m}. \text{ Right: } H > L; T_a = 1000 \text{ K}, \rho_a = 20 \text{ kg/m}^3, p_i = 200 \text{ MPa and } d_0 = 100 \mu\text{m}. \text{ Adapted from Ref. [72].} \]
The above has important implications for the complexity of spray models; when $H < L$, it is essential to include the radial coordinate of the spray in modeling, as is for instance done in the Valencia spray model, see section 8.4. In that case, the mutual influence between evaporation and combustion is obviously large, since the flame “surrounds” the liquid core.

Considering the mechanism of flame stabilization at $x = H$, there is still considerable debate. An explanation originally suggested by Kalghatgi [41] is that, at the flame base, the upstream turbulent burning velocity just balances the downstream convective spray velocity. This hypothesis was used in Ref. [72] to correlate the results, based on a theoretical relationship by Peters [60] derived from this hypothesis. However, it appears not to explain all observed trends. Specifically, it does not explain the observed large differences in $H$ between fuels (burning velocities of most fuels are very similar!).

An alternative explanation has been suggested by Pickett et al. [64], who convincingly establish a connection between the observed lift-off length and the ignition delay of the fuel. It comes down to assuming that $H$ establishes at a location where newly incoming fuel has had enough time to auto-ignite. This is confirmed by the observation of intermittent ignition pockets slightly upstream of $H$. The auto-ignition hypothesis seems to be confirmed by recent measurements in which forced ignition is applied [61], although the latter authors ascribe their observations to re-entrainment of hot combustion products, rather than auto-ignition. This mechanism is also mentioned in Ref. [64].

Clearly, the discussion on the stabilization mechanism of $H$ has not yet been finished. A recent suggestion is that, at the prevailing high temperatures in diesel engines, flame propagation chemistry and ignition chemistry become more similar, so there would be less of a contradiction than suggested above (Kalghatgi, private communication, 2010).

The equivalence ratio of the rich premixed flame near $x = H$ is generally between 2 and 4. The resulting products of incomplete combustion (partially oxidized fuel, CO and soot precursors) travel further downstream, in the hot core region of the spray, where ideal conditions for soot formation and growth exist [63]. The resulting soot and remaining products are subsequently oxidized for the largest part in the diffusion flame surrounding the spray – although “surrounding” may not be the right word; due to turbulence, the diffusion flame front is heavily distorted and wrinkled.

The diffusion flame is also the main location of NO formation (which in the exhaust pipe partly transforms into NO$_2$). The amount of NO is mainly governed by the adiabatic flame temperature $T_{\text{ad}}$. This in turn is mostly governed by in-cylinder conditions (intake temperature and EGR percentage), and is less affected by other fuel parameters or spray details.

From the above description it will be clear that the amount of exhaust-soot is very much affected by details of spray combustion. It has been shown that the amount of soot formed depends strongly on the equivalence ratio of the rich premixed flame $\phi(H)$. Whenever $\phi(H)$ is smaller than 2, no significant exhaust-out soot is observed [73, 49]. This might be tentatively explained by the hypothesis that, on average, each C atom oxidizes to CO when $\phi = 2$, thereby preventing it from going into soot precursor molecules.

If $\phi(H) > 2$, a strong correlation of its value with the amount of soot in the spray is observed [73]. This will be quantified more in section 8.2. However, the amount of exhaust-out soot in that case was recently found to be limited by oxidation rates rather than $\phi(H)$ [5].

Summarizing, the flame lift-off length $H$ is an important parameter for soot emissions, since it determines the amount of air entrainment upstream of the premixed flame, at the foot of the burning diesel spray. This will be further quantified in section 8.2.
3 Classification of spray models

In view of the enormous complexity of the spray process in engines, it will come as no surprise that many attempts have been made to provide simplified models of (parts of) the process. These models fall apart into different categories.

3.1 Heuristic models; correlations

The first and oldest category are empirical correlations, i.e. equations that are capable of reproducing experimental observations of sprays. Such models make no attempt to explain the observations; they merely describe them, although the chosen mathematical form is preferably based on some physical insights. Therefore, these models are named “heuristic” models, or just correlations. Examples were already shown in the previous section. Eqs. (18.6)-(18.9) were derived purely based on observations, without any attempt to explain the magnitude of the powers. The same holds for the correlation of Sauter mean diameters of droplets, Eq. (18.5).

Since correlations are often not more than curve fits (polynomial, exponential or power laws), they can only be used in the range where they have been fitted. As a matter of fact, this rule is often overlooked in practice. There are many examples of fits being “abused” outside their fitted range, and often this is hard to notice. CFD spray models often contain submodels in the form of empirical correlations, without clearly pointing out their limitations in the manual. However, this remark is not exclusive to spray modeling; it holds wherever descriptive models are used to make predictions.

As a matter of fact, a myriad of correlations has been used to describe macroscopic observations of sprays. As an illustrative example, one may look at Ref. [29]. By then, in 1985, already 21 different correlations for spray penetration were listed, 4 for SMD, 9 for cone angle and 9 for ignition delay. The needed parameters are not very well specified in that paper. Moreover, it must be noted that Ref. [29] is fairly old. More recent books, e.g. those of Stiesch [77] and Baumgarten [8] are good sources of more recent correlations. Still, in view of the fact they should always be used with care, empirical correlations are generally unattractive for studying spray combustion over broader parameter ranges. Especially when models are extrapolated to conditions that have not yet been tested – one of the main purposes of modeling! – one should be careful.

3.2 Phenomenological models

As a second class, phenomenological models are model descriptions based on some understanding of the underlying physics of the problem. However it is recognized that the physics can not be covered in full detail. Consequently, simplifying assumptions are made to make the model mathematically tractable.

As an example, for a spray, one can look at integral conservation laws to draw conclusions about the scaling of penetration with density or other parameters. The resulting models are often analytical or semi-analytical; that is, they can be expressed in a limited number of equations that can be solved using a pocket calculator or, at most, a simple computer (as opposed to CFD computations).

Phenomenological models are thus appealing, since they combine physical insight with computational simplicity. They also allow some (cautious) extrapolation, which enables parameter studies over wider parameter ranges (model-based extrapolation is far safer than using e.g. polynomials!). Last but not least, phenomenological models of evaporating fuel sprays can be used to provide source terms for the gas phase in CFD models, thereby avoiding the notorious grid dependency problems associated with “conventional” spray CFD models, which will now be discussed.
3.3 Computational Fluid Dynamics

A third and final category of spray models are those based on Computational Fluid Dynamics (CFD). In CFD modeling, the transport equations of mass, momentum and energy (and, in combustion systems, also species) are solved for every single cell in the computational grid. Therefore, far less simplification is needed. The associated drawback is, of course, that CFD models are by far the most demanding in terms of complexity and computation time.

Particularly for sprays, there are other complications at hand. As argued in, for example, Refs. [80, 39, 38, 77, 8], it is widely observed that the results of spray CFD modeling principally suffer from grid dependency. This holds both for the grid cell size and for the structure of the grid. The reasons are twofold: lack of spatial resolution in the vicinity of the nozzle, and lack of statistical convergence in the treatment of the liquid phase [8].

In order to do meaningful computations, the grid size should preferably be smaller than the typical nozzle dimension. Abraham [1] has shown that at least 4 grid cells should fit within the nozzle hole. The latter being of the order of 0.1 mm, this clearly forms a limitation for computations of practical sprays in realistic combustion chambers (with a size of the order of 0.1 m) – a difference of 3 orders of magnitude in length scale, which is 9 orders of magnitude in volume!

Moreover, it is very difficult to compute the complex two-phase phenomena inside a spray. Generally, the gas phase is computed in an “Eulerian” way, making use of a fixed grid. The liquid phase is kept track of in a separate (“Lagrangian”) model. Such Euler-Langrangian models are still the default approach [8]. Of course, mass, momentum and energy are exchanged between the two, which requires detailed knowledge both on the droplet population (size, temperature, velocity etc.) and the exchange mechanisms.

Moreover, the Lagrangian approach requires that the void fraction of each Eulerian cell is close to one, i.e. the fraction of liquid in each cell must be small (not larger than about 10%). This requirement is clearly not met for small grid cells in the immediate vicinity of the nozzle, which would be mostly filled with liquid. To get around it, grid cells are used that are sufficiently large, so as to reduce the amount of liquid in each cell in the vicinity of the nozzle. This is clearly in contradiction with the requirement of sufficiently small grid cells.

The result of the above is that the submodels used for spray vaporization become dependent of the grid size. To overcome this, it is common practice to tune parameters of submodels in order to give meaningful overall results. However, the resulting tuned parameters often do not have physically meaningful values any more. As Stiesch formulates it [77]: “submodels are trimmed to an unphysical behavior in order to overcome the deficiencies caused by inadequate grids”.

In recent years, a new approach has emanated which is able to overcome the grid dependency issue. In this so-called Euler-Euler approach, the liquid phase is no longer explicitly “followed”. Instead, both vapor and liquid phases are present within the same computational grid. This requires modeling of the vaporization process, in order to “distribute” the fuel in each cell over both phases. This can be done either in a “droplet-limited” or “mixing-limited” fashion.

Examples are the work of Abraham and Magi [2], Wan and Peters [81], Iyer et al. [39, 38] (who also provide a first exploration of the limits between both regimes) and of Versaevel, Motte and Wieser [80]. The latter authors present a mixing-limited model of spray vaporization that allows the use of an all-Eulerian model, with source terms based on a phenomenological model of the fuel spray. Their model will be covered in more detail in the section to come. In that section we will only discuss the submodels themselves; for the way of implementing them into CFD models, refer to the corresponding papers.
4 Phenomenological spray models

In this section the most important (semi-)phenomenological spray models will be discussed in more detail. The treatment will necessarily be concise – avoiding derivations and lengthy explanation, only mentioning the main points and equations. For more details the reader is referred to the original papers.

4.1 The Hiroyasu model

One of the first successful models of diesel spray combustion is the “package model” by Hiroyasu and coworkers. Introduced in 1976 [33], it was later extended and improved several times [34, 82]. In this model, a diesel spray is divided into a number of packages, each containing a fixed amount of fuel mass. The amount of air in each package changes due to air entrainment. A schematic picture is provided in Fig. 18.9.

![Figure 0.9: Schematic picture of Hiroyasu’s package model of spray combustion](image)

**Penetration**

Penetration of the spray tip $S(t)$ is described by

\[
S = 0.39 \sqrt{\frac{2\Delta p}{\rho_l}} \cdot t, \quad 0 < t < t_b \tag{22}
\]

\[
S = 2.95 \left(\frac{\Delta p}{\rho_a}\right)^{1/4} \sqrt{d_0 t}, \quad t \geq t_b \tag{23}
\]

where $t_b$, denoted as the *breakup time*, indicating the transition between the regimes dominated by liquid penetration and by air entrainment, is given by

\[
t_b = 28.65 \frac{\rho_l d_0}{\rho_a \Delta p}. \tag{24}
\]

The constants in the above equations can be generalized to account for a variable nozzle discharge coefficient $C_d$, as demonstrated by Jung and Assanis [40]. This results in replacing 0.39 with $C_d$ in Eq. (18.22) and replacing 28.65 with $4.35/C_d^2$ in Eq. (18.24). These authors also provide a very useful and detailed explanation of their implementation.
The above equations hold for the central packages of the spray. Corrections are provided for packages at the periphery, which move more slowly, and for the effect of swirl on penetration. These corrections can be found in the original papers and will not be reproduced here.

**Vaporization**

Air entrainment into each package is derived from momentum conservation: $m_f U_0 = (m_a + m_f) U$, resulting in

$$m_a = m_f \left( \frac{U_0}{dS/dt} - 1 \right).$$  

Hence, the air-fuel ratio in each package follows from the penetration speed of each package and the initial velocity $U_0$ at the nozzle. Again, corrections are made to this equation (by introducing simple correction constants) to account for the effects of ignition and wall impingement. For convenience, the differential air entrainment rate can be derived from Eq. (18.25), giving

$$\dot{m}_a = -m_f U_0 \left( \frac{dS}{dt} \right)^2 \frac{d^2S}{dt^2}.$$  

The fuel mass in each package can be combined with the Sauter Mean Diameter of the droplets (which follows from separate measurements, cf. [32]) to provide the number of droplets in each package. Given the air-fuel ratio of each package, droplet evaporation is then computed from the equations provided in section 6.4.

Liquid length is not explicitly addressed in the Hiroyasu model, although it can be obtained from following the packages on the central line and establishing the point in time (and, via $S(t)$, position) where the droplets have fully evaporated.

Historically, package models have always been combined with droplet-limited vaporization. However, there is no reason why mixing-limited vaporization could not be used in a package model. This would greatly simplify the model, since the amount of fuel evaporation for each package over time would in that case simply be obtained from a combination of air entrainment, described by Eq. (18.25), and thermodynamic equilibrium obtained from Eqs. (18.19) and (18.20), both for $m_v$ instead of $m_f$ as long as not all fuel has evaporated.

**Combustion**

The equivalence ratio $\phi$ in each package is obtained from the vaporized fuel mass, resulting from droplet evaporation, and the entrained air. The $\phi$ value of each package is used to predict soot and NO$_x$ emissions. For the latter, simple correlations (available by that time) were used, which are not reproduced here for reasons of brevity.

These correlations also involve temperature, which is obtained for each package taking into account evaporation and mixing (air entrainment). The ambient temperature $T_a$ is kept track of, taking into account the engine’s compression and expansion process, and heat loss to the cylinder wall. The latter is also described using empirical correlations. The same holds for the ignition delay $\tau_{ID}$, which identifies the time after which combustion sets in (i.e., auto-ignition is not modeled explicitly). Again, a similar approach is followed in Ref. [40].
4.2 The Sandia model

Penetration

Sandia researchers have developed a spray model that is able to correlate many of their measurements. A large database is available online, see https://share.sandia.gov/ecn/sprayCombustion.php. The model started with the work of Naber and Siebers on spray penetration [52], and was later extended to include liquid length [75] and equivalence ratio at lift-off [72]. Later it was used in an effort to correlate ignition delays to residence times for measured lift-off length [64]. Below the main equations are reproduced. Not all symbols are explained, since most of them have occurred earlier.

![Diagram of the Sandia spray model](https://example.com/sandia_diagram.png)

**Figure 0.10:** Schematic picture of the Sandia spray model with radially uniform profiles

In the derivation of the Sandia model, an idealized geometry is used, represented in Fig. 18.10. The idealized spray is characterized by constant composition and velocity over each cross-section at position $x$. The spray tip velocity is, within this model, assumed to equal the cross-sectional average velocity $v(x) = \frac{dx}{dt}$. Starting from fuel mass and momentum conservation, Naber and Siebers [52] derive an equation for the dimensionless spray tip velocity:

$$\frac{d\tilde{x}}{d\tilde{t}} = \frac{2}{\sqrt{1 + 16\tilde{x}^2} + 1}.$$

This equation can be analytically integrated to give

$$\tilde{t} = \frac{\tilde{S}}{2} + \frac{\tilde{S}}{4} \sqrt{1 + 16\tilde{S}^2} + \frac{1}{16} \ln\left(4\tilde{S} + \sqrt{1 + 16\tilde{S}^2}\right).$$

Dimensionless position $\tilde{x}$ (for spray tip: $\tilde{S}$) and time $\tilde{t}$ have been introduced, according to

$$\tilde{x} = \frac{x}{x^*}, \quad x^* = \frac{\rho_f}{\rho_a} \frac{\sqrt{C_a d_0}}{a \tan(\theta/2)}$$

$$\tilde{t} = \frac{t}{t^*}, \quad t^* = \frac{1}{U_0} \frac{\rho_f}{\rho_a} \frac{\sqrt{C_a d_0}}{a \tan(\theta/2)}$$

In these equations, spray cone angle correlations derived from the same set of measurements are used. For vaporizing conditions, these are given by Eq. (18.9). The observed values of $\theta$ are multiplied with a constant value $a$ to “compensate” for the effect of the idealized spray geometry.
The value of $a$ in Eq. (18.28) was first empirically fitted to 0.66, and later adjusted to 0.75 [73]. The latter value is in accordance with theoretical considerations, in which radial profiles of fuel mass and velocity are also considered. This is demonstrated in the appendix of Ref. [52]. (However, their Eq. (C23) is in error: both $A(x)$ and $A(x)$ should be omitted from it, as confirmed by Dennis Siebers in private communication). More importantly, it thus appears that the constant $a$ in a way accounts for the more realistic radial profiles in the spray. In section 8.4 we will see that the Valencia model explicitly takes these into account.

It can be shown that Eq. (18.28) reduces to the well-known limits $S \propto t$ for small values of $t$, and $S \propto \sqrt{t}$ for large $t$. The transition between these regimes occurs for $\tilde{t} \approx 1$. Since the equation is explicit in $\tilde{t}$ rather than $\tilde{S}$, it would often be easier to work with the inverse relation. This can however not be obtained analytically from Eq. (18.28); as an alternative, it is shown in Ref. [52] that the relation

$$\tilde{S} = \tilde{t} \cdot \left(1 + \tilde{t}^{2/2}\right)^{-1/n}$$

(31)

gives results very close to those of Eq. (18.28) for $n = 2.2$.

Vaporization

As in the Hiroyasu model, vaporization modeling must take into account air entrainment. As a spin-off from the penetration model, the fuel-air mass flow ratio at (dimensionless) position $\tilde{x}$ can be shown to obey

$$\frac{\dot{m}_f(\tilde{x})}{\dot{m}_a(\tilde{x})} = \frac{2}{\sqrt{1 + 16 \cdot \tilde{x}^2} - 1}.$$  

(32)

At the same time, again from thermodynamic considerations, the fuel-air ratio can be obtained from an enthalpy balance at the position where all liquid has just disappeared (i.e. the liquid length $L$). From that enthalpy balance, Siebers shows that

$$B \equiv \frac{\dot{m}_f(L)}{\dot{m}_a(L)} = \frac{h_a(T_a, p_a) - h_a(T_s, p_a - p_s)}{h_f(T_s) - h_f(T_f, p_a)} = \frac{p_s(T_s)M_f}{[p_a - p_s(T_s)]M_a} \cdot \frac{Z_a}{Z_f}.$$  

(33)

From the final equality, the saturation temperature $T_s$ can be obtained; the value of $B$ follows from the same computation.\(^1\)

Knowing $B$ and inserting it into Eq. (18.32) for $\tilde{x} = \tilde{L} = L/x^+$, it follows that

$$\tilde{L} = 0.25 \sqrt{\left(\frac{2}{B} + 1\right)^2 - 1}.$$  

(34)

In dimensional form,

$$L = \frac{b}{a} \sqrt{\frac{\rho_f}{\rho_a}} \cdot \sqrt{\frac{C_a}{\tan(\theta/2)}} \cdot \sqrt{\left(\frac{2}{B} + 1\right)^2 - 1},$$  

(35)

where the 0.25 has been substituted by constant $b$. The latter is tuned by Siebers in Ref. [75] to a value of 0.41. A more elaborate discussion on the model constants $a$ and $b$ is given in Ref. [45]. It turns out that, within the cross-sectionally averaged models, values obtained for $b$ are fairly constant [80]. However, the need of a tunable constant is a serious shortcoming of the model. In the Valencia spray model, using radial distributions of fuel vapor fraction and velocity, it appears that such constants are not needed to achieve satisfactory agreement with measured liquid lengths [16].

\(^1\)The ratio of compressibility factors appearing at the end of Eq. (18.33) is an – actually wrong – attempt to account for real gas effects. In Ref. [45] it is shown how this can be done more consistently. The same holds for the pressure dependency of the enthalpy terms in this equation.
Combustion

From Eq. (18.32), the fuel-air ratio is – in principle – known at every position \( x \). However, this ratio pertains to the total fuel content, not only the vapor. Downstream of the liquid length, fuel only exists in vapor phase, and in that case the fuel-air ratio of Eq. (18.32) equals that of the vapor phase. In section 6 we have seen that, for modern diesel conditions, the flame lift-off \( H \) is often larger than \( L \). In that case, we can use the fuel-air ratio at \( H \) to estimate the local equivalence ratio:

\[
\phi(H) = \frac{2AF_s}{\sqrt{1 + 16(H/x^+)^2} - 1}.
\]

As discussed in section 6, the equivalence ratio at \( H \) has important consequences for soot formation. Whenever \( \phi(H) < 2 \), no significant soot formation is found. This was hypothetically attributed to every C-atom being bound to 1 oxygen atom.

This observation was later extended [48] to include oxygenated fuels, introducing the total atomic oxygen ratio \( \Omega \). The latter is a combination of fuel oxygen and the “conventional” equivalence ratio, and accounts for the total amount of available oxygen with respect to stoichiometric:

\[
\Omega(H) = \frac{1 - \Omega_f}{\phi(H)}.
\]

In this equation, \( \phi \) is the equivalence ratio resulting from air entrainment. \( \Omega_f = z/(2x+y/2) \) represents the amount of oxygen available in the fuel, over the amount that is stoichiometrically needed for an oxygenated fuel characterized by \( C_xH_yO_z \). It appears that all fuels tend to zero soot when \( \Omega \) becomes larger than 50%. However, the initial soot level (and thus the slope) differs per fuel [62, 48], as depicted in Fig. 18.11, adapted from Ref. [48].

![Image](image.png)

**Figure 0.11**: Observed soot versus total atomic oxygen ratio at flame lift-off \( \Omega(H) \), adapted from Ref. [48]

The above method of predicting local equivalence ratios was first used explicitly for combustion modeling by Flynn et al. [25]. They divided the combusting spray into zones of varying temperature and equivalence ratio, and applied detailed chemical kinetics for each zone. Although this approach was still rather crude, it did explain some of the observed trends in soot formation. Their Figs. 10 and 16 (not reproduced here) nicely summarize their main findings.

In recent years, the Sandia model has been used by many authors. As an example, the work of Bayer and Foster is mentioned [9], who combine the above model with simple emission formation models (very similar to those employed earlier by Hiroyasu and coworkers [34, 82]) to compare with experimental engine data.
4.3 The Versaevel model

The Sandia liquid length scaling law, summarized in the previous section, only provides information on the liquid length position. No information is available on the evaporation (hence fuel content of the mixture) upstream of \( L \). This point has been addressed by Versaevel, Motte and Wieser [80].

Introducing the void fraction \( m \), they account for vaporization upstream of \( L \). This is done assuming mixing-limited vaporization at any position \( x \) upstream of \( L \), not only for \( L \) itself. The model is embedded in the same context as the Sandia model, being an idealized spray with radially uniform fuel fraction and velocity profiles (as depicted in Fig. 18.10).

Introducing the mass flow ratio \( \Delta \) (equivalent to \( 1/B \) in the Sandia model), Versaevel et al. derive from fuel mass conservation:

\[
\Delta = \frac{\dot{m}_f}{\dot{m}_f^0} = \frac{m(1 - Y_{fg})p_g}{\rho_f(1 - m) + mY_{fg}p_g},
\]

where \( Y_{fg} \) is the mass fraction of fuel in the gaseous phase. The parameter \( \rho_g \) represents the density of the gaseous mixture, containing fuel vapor and ambient gas.

From total momentum conservation, a similar expression follows:

\[
\Delta^2 = \frac{Am^2(1 - Y_{fg})^2\rho_g^2}{A_0\rho_f[1 - m]\rho_f + m\rho_g^2].
\]

The surface area ratio \( A/A_0 \) is fully determined by geometry. For each position \( x \), its value equals \( A/A_0 = 1 + (2x/d_e)a\tan(\theta/2) \), with \( d_e = \sqrt{C_d d_0} \).

The law of energy conservation in this framework reads

\[
\dot{m}_f^0h_f(T_f) + \dot{m}_a h_a(T_a) = \rho_f(1 - m)A\dot{v}h_f(T) + Y_{fg}\rho_gmA\dot{v}h_{fg}(T) + \dot{m}_a h_a(T),
\]

which can be rewritten in terms of specific heats as

\[
\Delta \int_T^{T_a} c_{pa}(s)ds = \left( \frac{Y_{fg}\Delta}{1 - Y_{fg}} - 1 \right)L_a(T) + L_a(T_f) + \int_{T_f}^T c_{pf}(s)ds.
\]

Herein \( c_{pa} \) is the specific heat of the entrained ambient gas and \( c_{pf} \) that of the fuel vapor. \( L_a \) represents the latent heat of vaporization. \( T \) denotes the temperature of the gas-vapor mixture at axial position \( x \).

The three basic conservation laws (18.38), (18.39) and (18.41) contain the unknowns \( \Delta, m, \rho_g, Y_{fg} \) and \( T \). Upstream of the liquid length, the assumption of thermodynamic equilibrium couples the mass fraction of fuel vapor to temperature. The fuel partial pressure equals the fuel saturated vapor pressure: \( X_{fg} = p^r/p_a \), where \( X_{fg} \) is the saturated fuel molar fraction. Converting it to a mass fraction – notice the similarity with Eq. (18.20) – gives

\[
Y_{fg} = \frac{1}{\left( \frac{p_a}{p(T_f)} - 1 \right)M_f/M_g + 1}.
\]

Assuming uniform pressure, \( \rho_g \) can be linked to \( T \) and \( Y_{fg} \) via the ideal gas law, yielding

\[
\rho_g = \rho_a\frac{T_a}{TY_{fg}M_g/M_f} + [1 - Y_{fg}].
\]

Using the three non-linear conservation equations (18.38), (18.39) and (18.41), and aided by Eqs. (18.42) and (18.43), the unknowns \( (T, \Delta \) and \( m) \) can be found using standard numerical methods. Downstream of the liquid length, the void fraction \( m \) is unity and \( Y_{fg} \) becomes smaller than its saturated value, due to continuous air entrainment. As a result, Eq. (18.20) is no longer valid, and \( Y_{fg} \) becomes an unknown in Eqs. (18.38), (18.39) and (18.41), with \( m = 1 \) in that case.
Penetration

An excellent description of the Versaevel model and its implementation is given by Bekdemir [10]. He also indicates how, from the obtained solutions sketched above, the velocity \( v(x) \) can be obtained. This is not trivial, since the model in principle provides quasi-steady solutions at each position \( x \). As in the Sandia model, the spray tip velocity is assumed to equal \( v(x) \). Hence, \( S(t) \) follows from integration of \( v(x) \), keeping track of the tip position:

\[
S(t + dt) = S(t) + v[S(t)]dt.
\] (44)

As also indicated by Bekdemir, the results of the model strongly depend on the chosen spray angle that needs to be put in. Versaevel et al. use the same spray angle correlation – Eq. (18.9) – as Siebers [75], effectively multiplied with the same constant \( a \) to account for the effect of the (unrealistic) idealized spray with cross-sectionally uniform variables.

Vaporization

The liquid length in the Versaevel model follows from the model results as the position where \( m = 1 \) first occurs. In principle, vapor and liquid penetration are computed simultaneously in this model. However, in order to achieve correspondence with liquid length data from Verhoeven et al. [79], the product of model constants \( ac \) needs to be adjusted from 0.23 to 0.104 (\( c = 0.27 \), see Eq.(18.9)) for liquid length computations. The authors argue that this is in accordance with the Sandia model, which also needs a specific correction factor \( b \) to achieve correspondence with experimental data.

Consequently, the model is run twice, with different values of \( ac \). The smaller value of \( ac \) provides the steady liquid length \( L \); the larger value provides transient penetration. Since vapor and liquid are known to penetrate together during the transient phase, the total liquid penetration \( x_l \) is evaluated as

\[
x_l(t + dt) = \min(S(t + dt), L).
\] (45)

Although the resulting constants of the Sandia and Versaevel models are indeed equivalent [80, 45], it appears that liquid length results are not the same [10]. Luijten and Kurvers [45] provide an in-depth analysis of the differences between the models. In doing so, they derive a closed expression for the liquid length in the Versaevel model:

\[
L = \frac{1}{4a} \sqrt{\frac{\rho_a(L)}{p_a(L) \tan(\theta/2)}} \left[ \frac{2}{B} + 1 \right]^{1/2} - 1 - \frac{1}{2a} \frac{\sqrt{C_a d}}{\tan(\theta/2)}.
\] (46)

This equation bears great similarity to Eq. (18.35). Apart from the (small) last term, which corrects for the effect of finite nozzle size, the main difference is in the evaluation of \( \rho_a \). In Eq. (18.46) it is evaluated at \( L \), with temperature \( T_s \) instead of \( T_a \). Physically, this difference accounts for the effect of upstream vaporization on penetration. Although at \( x = L \) a considerable amount of fuel vapor is present, lowering the partial density of air, the temperature effect is dominant. The result is a higher \( \rho_a \) value, and hence smaller liquid lengths.

Another important conclusion from Ref. [45] is that the thermodynamics in both models are fully equivalent, i.e. the same values of \( B \) resp. \( 1/\Delta \) and \( T_s \) are found. This confirms the earlier conjecture that the saturation thermodynamics can be decoupled from the process of spray penetration, which is purely governed by dynamics. Still, the above argument suggests that there can be a one-way coupling from thermodynamics to spray penetration. This needs to be investigated further.
**Combustion**

The Versaevel model was introduced to avoid the notorious grid dependency problems with Euler-Lagrangian spray models. The model introduces source terms of fuel mass, momentum and energy into an Eulerian CFD model of the gas phase. This is done only for the region up to the liquid length $L$; after that region, the CFD model takes over (the source terms become zero anyway for $x > L$).

Bekdemir [10] has investigated this approach more closely and writes down the resulting source terms explicitly. The time derivative of liquid fuel mass is

$$
\dot{m}_{fl}(x) = \rho_{fl}[1 - m(x)]A(x)v(x),
$$

where all quantities can be obtained from the spray model. Division by a volume element $A(x)\,dx$ and changing the sign gives the source term of fuel vapor mass per unit of time and volume:

$$
\dot{m}_{fv} = -\frac{1}{A(x)} \frac{d\dot{m}_{fl}(x)}{dx}.
$$

(47)

Similarly, the momentum source term is obtained from multiplying Eq. (18.47) by $v(x)$:

$$
\dot{M}_{fv} = -\frac{1}{A(x)} \frac{d(\dot{m}_{fl}(x)v(x))}{dx}.
$$

(48)

The energy source term is slightly more complex, since energy is transferred in both ways. A negative enthalpy source term represents liquid heating, whereas a positive one accounts for added fuel vapor:

$$
\dot{E}_g(x) = -\frac{1}{A(x)} \frac{d\dot{E}_{fl}}{dx} + \dot{m}_{fv}E_{fg}(x),
$$

(50)

where $E_i = h_i - p_i/\rho_i(x) + v(x)^2/2$ with $i = f, g$ for both phases.

Using this approach, Bekdemir [10] was able to couple the Versaevel model to a commercial CFD code. Combustion can then be modeled using any method of choice; this is fully decoupled from the spray model, since the latter only affects gas phase composition and temperature. For this reason, combustion modeling is not further addressed here. An example result is shown in Fig. 18.12.

![Figure 0.12: Temperature contours of combusting n-heptane spray, using two different combustion models (eddy-dissipation model and FGM). Taken from Ref. [10]. Notice the different flame-lift off positions](image)
4.4 The Valencia model

In this section the spray model, developed over the last decade at the Universidad Politécnica de Valencia, is discussed. Like the models discussed above, it is semi-phenomenological in nature; i.e. not solving the full 3D equations, but simplifying the physics to an extent that overall relations can be deduced for e.g. spray tip penetration and liquid length. This enables to establish relations between these phenomena and, for instance, density, temperature, injection pressure and nozzle characteristics.

Concerning the latter, the same group has published a lot of work on the determination of nozzle characteristics and their effect on spray development. An important general conclusion of that work is that nozzle details, via the spray cone angle, play a very essential role in prediction of macroscopic characteristics. Therefore, generalization of modeling results is very hard without measuring nozzle discharge characteristics $C_d$, $C_a$ and $C_v$, cf. Ref. [6].

To connect to the models discussed earlier, it helps to realize the following. Both the Sandia and Versaevel models are able to compute certain properties for every $x$-position in the spray. It might seem that this is only possible due to the assumption that these properties are uniform over each cross-section; however, if the functional form of the radial profile is prescribed, it is possible to obtain radial profiles from integral conservation laws.

More specifically, Gaussian profiles are used; besides allowing easy integration, a physical reason for this lies in the Central Limit Theorem. This states that a combination (convolution) of many arbitrary statistical distributions will always give an overall Gaussian profile. Also experimentally, Gaussian profiles are always observed for velocity and fuel mass distribution.

Penetration

The Valencia spray penetration model, first published in Ref. [21], starts from conservation of momentum for every position $x$:

$$
\dot{M}(x) = \dot{M}_0 = \int_0^R 2\pi \rho(x, r) r U^2(x, r) dr.
$$

(51)

The momentum flow $\dot{M}_0$ at the nozzle is an input to the model (and can be measured as discussed before). The velocity field is prescribed as

$$
U(x, r) = U_{axis}(x) \exp \left[-\alpha \left(\frac{r}{R}\right)^2\right].
$$

(52)

The shape factor $\alpha$, related to the (measured) spray angle via the outer radius $R = x \tan(\theta/2)$, describes the radial width of the velocity profile. Taking $U(x, R) = 0.01 U_{axis}$, its value is 4.6. In principle, this self-similar velocity profile only holds in the conical (quasi-steady) part of the spray, constituting about 70-80% of the spray length.

The density in Eq. (18.51) complicates the integration. Therefore, in Ref. [21] a transformation is done to an iso-density spray, having the same exit velocity and momentum flux, but with a (larger) effective diameter $d_{eq} = d_0 \sqrt{\rho_f/\rho_a}$. In that case integration is straightforward and results in

$$
\dot{M}_0 = \rho_a \frac{\pi}{2\alpha} U_{axis}^2(x) \left[1 - \exp(-2\alpha)\right] x^2 \tan^2(\theta/2).
$$

(53)

In view of the large value of $\alpha$, the factor in square brackets can be omitted. The resulting axial velocity profile is

$$
U_{axis} = \sqrt[3]{\frac{\dot{M}_0^{1/2}}{\rho_a^{1/2}(\pi/2\alpha)^{1/2} x \tan(\theta/2)}}.
$$

(54)
Based on experimental as well as theoretical evidence, it is argued that the spray tip moves with a velocity equal to one-half of the expected axial velocity at \( x = S \), in other words \( dS/dt = 0.5U_{axis}(S) \). Since \( U_{axis}(S) \propto 1/S \), this can be integrated, resulting in

\[
S = \left( \frac{2\alpha}{\pi} \right)^{1/4} M_0^{1/4} \rho_a^{-1/4} t^{1/2} \tan^{-1/2}(\theta/2). \tag{55}
\]

From this result it appears that only the “square root limit” of \( S(t) \) is described. Although the authors recognize that there is a (short) period where penetration is linear with time, they make no attempt to model that; it is ascribed to the opening behavior of the nozzle, rather than a different flow regime [22].

In a later paper [19], the iso-density assumption is abandoned. Instead, a Gaussian profile is posed for the (total gas plus liquid) vapor fraction as well:

\[
Y_f(x, r) = Y_{f, axis}(x) \exp\left[ -\alpha Sc \left( \frac{r}{R} \right)^2 \right]. \tag{56}
\]

The density \( \rho(x, r) \) straightforwardly follows from this profile. Yet, this results in considerable mathematical complexity. However, if one assumes \( Sc = 1 \) and \( \rho_f \gg \rho_a \) (the resulting errors are quantified in Ref. [19]), the resulting expression is not too complex:

\[
M_0 = \frac{\pi}{\alpha} x^2 \rho_a \tan^2(\theta/2) U_0 \left[ -U_{axis} - U_0 \ln \left( 1 - \frac{U_{axis}}{U_0} \right) \right]. \tag{57}
\]

As before, \( U_{axis} \) can be solved from this equation, in this case by iteration. For \( Sc = 1 \) it can also be shown [21] that \( Y_{f, axis} = U_{axis}/U_0 \), in other words: the profiles of dimensionless velocity and mass fraction are identical. Consequently, having obtained \( U_{axis} \) as above, both \( U(x, r) \) and \( Y_f(x, r) \) are known.

Vaporization

The distributions of velocity and overall fuel mass fraction in the previous section were derived for an isothermal (i.e., non-vaporizing) spray. Evaporation complicates the problem further. Still, assuming mixing-limited vaporization, only equilibrium considerations are needed to solve the problem.

For \( Le = 1 \), the law of energy conservation (in terms of relative enthalpy) has exactly the same form as those for fuel mass and momentum. Therefore, without extra effort, the distribution of relative enthalpy throughout the spray is obtained. When also \( Sc = 1 \), we have:

\[
\frac{h(x, r) - h_{a,\infty}}{h_f(T_{f,0}) - h_{a,\infty}} = \frac{U(x, r)}{U_0} = Y_f(x, r) = Y_{f,\ell} + Y_{f,v}. \tag{58}
\]

For combustion modeling purposes the enthalpy field needs to be converted to temperature, which requires knowledge on the distribution of fuel over the (vapor and liquid) phases. Assuming mixing-limited evaporation, the distribution of fuel over the phases can be readily computed.

If \( Y_f \) is known everywhere, Eq. (18.58) provides a relation between \( T(x, r) \) and \( Y_{f,v} \). Inserting \( h = Y_f h_{f,\ell} + Y_{f,v} h_{f,v} + (1 - Y_f) h_a \) and \( h_{f,v}(T) = h_{f,\ell}(T) + \Delta h_{vap}(T) \) it can be rewritten as

\[
Y_{f,v} = \frac{(1 - Y_f)[h_a(T_a) - h_a(T)] - Y_f[h_{f,\ell}(T) - h_{f,\ell}(T_{f,0})]}{\Delta h_{vap}}. \tag{59}
\]

An extra relation between \( Y_{f,v} \) and \( T \) follows from the saturation condition:

\[
Y_{f,v} = \frac{M_f}{M_a} (1 - Y_f) \left( \frac{1}{X_{f,v} - 1} \right), \tag{60}
\]
where $X_{f,v}$ is the saturated molar fuel fraction in the gas phase (notice the difference with $Y_{f,v}$, which is the fuel vapor mass fraction in the mixture). In an ideal gas approximation, $X_{f,v} = p^s(T)/p_a$. In Ref. [16] it is shown how this changes in a real gas context. An easier formulation of the latter, in terms of enhancement factors, can be found in Ref. [45].

As in the Versaevel model, division of fuel over vapor and liquid phases is only relevant for the upstream/inner part of the spray. There, the above two equations are both needed to solve for $Y_{f,v}$ and $Y_{f,l}$. More downstream (and, in this case, also further to the spray edges), only fuel vapor is present. At the border of those regions, all liquid fuel has just evaporated. This contour is characterized by a temperature $T_{evap}$ and by one particular mass fraction $Y_{f,evap}$ which in that case equals $Y_f$ and $Y_{f,v}$. Inserting this into Eq. (18.59) gives

$$
\frac{Y_{f,evap}}{1 - Y_{f,evap}} = \frac{h_a(T_a) - h_a(T_{evap})}{h_{f,l}(T_{evap}) + \Delta h_{vap}(T_{evap}) - h_{f,l}(T_0)},
$$

which can be proven to be equivalent to $B$ in Eq. (18.33) and to $1/\Delta$ in the Versaevel model, with the same saturation temperature $T_{evap} = T_s$.

One issue not yet addressed above, is the effect of evaporation on density (via temperature). As we saw in the Versaevel model, this does affect spray penetration. For a vaporizing spray, the local density is given by

$$
\rho = \frac{1}{\frac{Y_{f,l}}{\rho_{f,l}} + \frac{Y_{f,v}}{\rho_{f,v}} + \frac{Y_a}{\rho_a}},
$$

where all parameters depend on $x$ and $r$. In this way, a coupling exists with the penetration law derived before: evaporation affects density, which in turns affects the distribution of $U/U_0$ and $Y_f$. In Ref. [16] this is stepped over rather loosely, making use of a simple scaling model for $Y_{f,axi}$. In a later paper [55] this coupling is accounted for in a self-consistent way. Consequently, the model is no longer analytically solvable (mainly since the coupling between $Y_{f,v}$ and $\rho$ is non-linear), and a numerical approach is used. This opens the way to take into account transient behavior (and deal with time-variant boundary conditions) and the effect of non-unity Sc number. Yet the model is still 1D, and therefore “on the verge between phenomenological and CFD modeling”.

An important advantage of the Valencia spray evaporation model is that it does not need any adjustable constants in order to correlate experimental penetration and liquid length data. Still, it remains questionable whether this also holds when comparing with other data sets than their own – often, best agreement is found with in-house data [75, 80, 18].

Combustion

Recently, Desantes et al. have extended the model of Ref. [55] to reacting sprays [17]. This is done by interpreting the fuel mass fraction $Y_f$ as a mixture fraction during combustion. Combustion is modeled using a one step irreversible reaction. Another change is in the state relationships, from which local density and temperature are obtained. With combustion, these relations necessarily must include the effect of chemical enthalpy (but including that is straightforward) and more species being present.

Overall, the approach remains very much the same as for non-reacting sprays, which is elegant. The work bears some similarity to that of Flynn et al. [25], who also use a physical spray model to compute the temperature/equivalence ratio field and then continue with combustion modeling in a phenomenological fashion.
5 Recent developments and Outlook

In this section some points are briefly sketched that are currently attracting attention.

Generally, there is a need for spray models that are capable to predict the penetration, evaporation and combustion behavior of sprays, including the formation of emissions. The approach of using semi-phenomenological models to provide source terms in CFD, thereby avoiding the inherent difficulties of Euler-Lagrangian models, seems to be the most promising.

Within the group of phenomenological models, the Valencia model seems the most promising. It is certainly more physical (including radial variations) and more accurate than the Sandia-based models, since no adjustable constants are needed to match the results with experimental data. On the other hand, the Versaevel model has also proven its ability to provide a CFD code with reasonable source terms. The CFD code rapidly translates the “artificially flat” source terms of the Versaevel model into radial variations [10]. If the flame lift-off length is sufficiently large, including the radial direction in the source term might not be needed. Yet, the Valencia model is expected to give better radial distributions from the start. It must be investigated whether this makes a significant difference in the combustion phase.

The above goal of accurate prediction of spray behavior should be accomplished over an extremely wide range of (often multi-component) fuels, bringing about a variety of fuel properties and injection conditions. Amongst these are extremely high pressures and various nozzle geometries. This is directly related to the large variety of fuels that is claiming a role on the future fuel market. Examples are biodiesel (with pure plant oils as an extreme case) and lighter molecules such as DME and ethanol.

Multi-component vaporization in sprays has been studied, amongst others, by Canaan et al. [12], Siebers [74] and Myong et al. [51]. Usually it is found that steady liquid length is dominated by the least volatile component in a mixture; more specifically, it is found to correlate well with $T_{90}$, the 90% boiling point of the mixture. Recently, Pastor et al. have correlated liquid length results for biodiesel blends in terms of mixing-limited vaporization [56].

Real gas effects in droplet-limited vaporization models were addressed, for instance, by Curtis et al. [13] and Hohmann et al. [35]. Real gas effects in mixing-limited models were investigated recently by Desantes et al. [16] and by Kurvers and Luijten [44, 45]. One aspect investigated in Ref. [45] is the interaction between spray penetration and vaporization in the models of Refs. [75] and [80]. It appears that mixture thermodynamics is decoupled from the spray penetration. The other way around, it seems that vaporization does affect the spray penetration speed, as reported in Refs. [80, 55]. This requires further investigation.

An extreme situation of real gas effects happens when the fuel enters the combustion chamber under conditions close to the critical point. When the fuel-ambient mixture immediately reaches the critical line, this results in flash boiling: the liquid phase instantly disappears by vigorous rupture. Although it might seem that every diesel spray would encounter supercritical conditions in the cylinder, this is not the case. In an excellent review on supercritical droplet vaporization, Givler and Abraham [26] show that the ambient pressure should be twice the fuel’s critical pressure and its temperature should be twice the fuel’s critical temperature, in order for the droplet to reach supercritical conditions before complete vaporization.

The conditions under which the assumption of mixing-limited vaporization may be used, are not yet established very well. An attempt in this direction by Iyer et al. [39] has not been fully convincing yet, and is not really quantitative in terms of where the boundary of mixing-limited vaporization is. It is recommended to investigate this transition by implementing the detailed droplet vaporization model sketched in section 6.4 into, for instance, the Valencia penetration model.
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