REAL GAS EFFECTS IN MIXING-LIMITED DIESEL SPRAY VAPORIZATION MODELS

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The maximum penetration length of the liquid phase in diesel sprays is of paramount importance in reducing diesel engine emissions. Quasi-steady liquid length values have been successfully correlated in the literature, assuming that mixing of fuel and air is the limiting step in the evaporation process. Since fuel injection in engines takes place at high pressure, nonideal gas effects may significantly affect the phase equilibrium. In this work, real gas effects are implemented into the mixing-limited spray vaporization models of Siebers and of Versaevel et al., taking into account enhancement of the fuel-saturated vapor pressure by the high-pressure ambient gas. Results show that this effect is significant at ambient densities relevant for diesel combustion. The effect of gas pressure on mixture enthalpy (and thereby on liquid length) is also considered but found to be negligible for relevant diesel conditions. Since both models discussed are based on almost the same premises but give different results, their intrinsic differences are evaluated by deriving a new closed-form expression for the Versaevel model. It is shown that the models can be “equalized” by adding a correction factor to the Siebers model, making it physically more consistent. However, for the (limited) data set considered in this paper, this does not improve its predictive capability. It is argued that the remaining error in model predictions is most probably due to the cross-sectional averaging approach.

KEY WORDS: diesel spray, real gas effects, equation of state, liquid length

1. INTRODUCTION

Direct injection diesel engines are widely in use, mainly because of their low fuel consumption and high specific power. Nowadays it is also needed to meet stringent emission regulations, while preserving power output. For direct injection diesel engines this means that the vaporization and combustion process of the fuel spray should be well understood.

Key parts in the diesel process are the penetration and vaporization of the liquid fuel spray. Especially, knowledge of the maximal penetration of liquid fuel into the cylinder (often referred to as the “liquid length”) is very important to avoid wall wetting, which can lead to unacceptable emission levels. The liquid length is also important to understand the general behavior of a combusting fuel spray; several regimes can occur, depending on whether the liquid length is shorter or longer than the flame lift-off length (Siebers and Higgins, 2001).

Liquid lengths can be predicted using semi-phenomenological spray models. These models can be divided into two categories. In droplet-limited vaporization models, the overall vaporization rate is governed (i.e., limited in time) by interphase transport at the droplet surface. Most of these models are based on the excellent work of Abramzon and Sirignano (1989). In mixing-limited vaporization models, it is assumed that these local processes are much faster than the global mixing rate of fuel and air. Effectively, this implies that droplets are in thermodynamic equilibrium with their surroundings at all times.

Mixing-limited vaporization models give quite accurate predictions of liquid lengths at normal engine condi-
The reason is that they are generally calibrated on experimental data retrieved at conventional (i.e., near top dead center) diesel engine conditions (Pickett, 2007). At other engine conditions, for example, at lower in-cylinder temperatures (of interest for early injection strategies), these models are less accurate (Boot et al., 2007). A conjecture lying at the basis of the present work is that this deficient predictive capability might be due to effects of nonideal gas behavior in the fuel-ambient gas mixture. Since fuel injection in engines typically takes place in a high-pressure environment, real gas effects could play an important role. This is especially true for ambient conditions not too far from the critical point of the injected fuel. The importance of real gas effects in droplet-limited spray models has been assessed by several authors (see, for instance, Curtis et al., 1995; Hohmann et al., 1996; Varanavas and Assanis, 1996; and Hohmann and Renz, 2003). The results of these authors typically show a significant impact of real gas effects on the evaporation of single droplets. Nevertheless, their effect on the overall spray behavior is found to be limited, sometimes attributed to a high evaporation rate in combination with a wide droplet size distribution.

The importance of real gas effect in mixing-limited vaporization models has not sufficiently been investigated so far. Although Siebers (1999) does address real gas effects in his original paper on liquid length scaling, his method is actually not correct, as we demonstrate in the next section. In the model by Versaevel et al. (2000), which is basically an extension of the Siebers model, real gas effects are not considered at all. Desantes et al. (2007) include real gas effects, based on the Peng-Robinson equation of state, in their thermodynamic state relationships. These are then inserted into a spray penetration model (derived for gas jets), which is assumed not to change due to fuel evaporation. Yet, they provide no systematic comparison between liquid length model results with and without real gas effects; such a comparison is only made for the saturated vapor mass fraction $Y_{f, evap}$. Finally, these authors use ideal gas enthalpy throughout their model (just as Siebers and Versaevel et al. do). Although results later in this paper provide justification for this, this approach cannot be assumed valid upfront.

The aim of the present study is to systematically assess the importance of real gas effects on the liquid length pre-

<table>
<thead>
<tr>
<th>NOMENCLATURE</th>
<th>Greek Symbols</th>
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<tbody>
<tr>
<td>$A$ cross-sectional area $[m^2]$</td>
<td>$\alpha$ idealized spray angle $[\text{rad}]$</td>
<td>$0$ initial and/or at nozzle exit</td>
</tr>
<tr>
<td>$a, b, c$ fit parameters $[-]$</td>
<td>$\Delta$ mass flow rate ratio $[-]$</td>
<td>$a$ ambient gas</td>
</tr>
<tr>
<td>$B$ mass flow rate ratio $[-]$</td>
<td>$\theta$ measured spray angle $[\text{rad}]$</td>
<td>$e$ effective</td>
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<tr>
<td>$C_a$ area contraction coefficient $[-]$</td>
<td>$\rho$ density $[\text{kg/m}^3]$</td>
<td>$f$ fuel</td>
</tr>
<tr>
<td>$c_p$ isobaric specific heat $[\text{J/kg K}]$</td>
<td>$\sigma$ standard deviation $[%]$</td>
<td>$g$ gaseous phase</td>
</tr>
<tr>
<td>$d$ orifice diameter $[m]$</td>
<td>$\varphi$ fugacity coefficient $[-]$</td>
<td>$i$ component index</td>
</tr>
<tr>
<td>$f_e$ enhancement factor $[-]$</td>
<td></td>
<td>$l$ liquid phase</td>
</tr>
<tr>
<td>$h$ enthalpy $[\text{J/kg}]$</td>
<td></td>
<td>$L$ liquid length</td>
</tr>
<tr>
<td>$L$ liquid length $[m]$</td>
<td></td>
<td>$s$ saturation</td>
</tr>
<tr>
<td>$L_v$ heat of vaporization $[\text{J/kg}]$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m$ void fraction $[-]$</td>
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<tr>
<td>$M$ molar mass $[\text{kg/mol}]$</td>
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<tr>
<td>$\dot{m}$ mass flow rate $[\text{kg/s}]$</td>
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<tr>
<td>$p$ pressure $[\text{Pa}]$</td>
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<tr>
<td>$R$ gas constant $[\text{J/(mol K)}]$</td>
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<td></td>
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<tr>
<td>$T$ temperature $[\text{K}]$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$v$ velocity $[\text{m/s}]$</td>
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<td></td>
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<tr>
<td>$x$ axial coordinate $[m]$</td>
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<td></td>
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<tr>
<td>$x^+$ length scale $[m]$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\tilde{x}$ dimensionless coordinate $[-]$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$X$ mole fraction $[-]$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$Y$ mass fraction $[-]$</td>
<td></td>
<td></td>
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<td>$Z$ compressibility factor $[-]$</td>
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**Sub-/Superscripts**

- $0$ initial and/or at nozzle exit
- $a$ ambient gas
- $e$ effective
- $f$ fuel
- $g$ gaseous phase
- $i$ component index
- $l$ liquid phase
- $L$ liquid length
- $s$ saturation

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dictions of two mixing-limited spray vaporization models. This holds both for the impact of nonideal gas enthalpy relations and of the enhanced saturated vapor pressure of a fuel when exposed to a high pressure of ambient gas. A second objective of the paper is to carefully examine the differences between these two models, which both assume radially uniform velocity and concentration profiles over the spray.

The structure of this paper is as follows. Section 2 first briefly describes the Siebers (1999) and Versaevel et al. (2000) models. Then we describe how real gas effects can be implemented in both. Section 3 presents results of both the original and modified (i.e., real gas) models. We also shed more light on the mutual differences between the models themselves. In doing so, we present a closed-form expression for the model by Versaevel et al. Its derivation is presented in the Appendix.

2. THEORY

In this section, first the Siebers liquid length model is summarized. Essential steps in the derivation are reproduced, mainly with the aim of providing insight into the differences with the Versaevel model. The latter is described in Section 2.2. Section 2.3 describes how real gas effects can be properly taken into account in both models.

2.1 Siebers’ Liquid Length Scaling Model

A scaling model for liquid length, based on the assumption of mixing-limited vaporization, was first presented by Siebers (1999), based on a large database of measured liquid lengths (Siebers, 1998). It is derived using integral control surface techniques in combination with an idealized model of the quasi-steady phase of a diesel spray (see Fig. 1, reproduced with permission).

Liquid fuel is injected from the nozzle and forms a spray with idealized angle $\alpha$. At the left side of the control volume the spray contains only liquid fuel with temperature $T_f$ and density $\rho_f$. At the right side of the control volume (i.e., at the liquid length $L$) all liquid has just vaporized. Upstream of the liquid length, ambient gas with temperature $T_a$ and density $\rho_a$ is entrained, causing the liquid fuel to heat and vaporize. At $x = L$ the temperature and density are a priori unknown. The pressure $p_a$ is uniform throughout the spray.

Using this idealized model, Siebers derives a liquid length expression based on conservation of (fuel) mass, momentum, and energy. Only the essential steps are reproduced here, for the sake of argumentation in Section 2.3.

Assuming uniform velocity over each radial cross section and no slip between fuel and ambient gas within the spray, the ratio of mass fluxes at $x = L$ equals the ratio of partial densities $\rho_a$ and $\rho_f$:

$$\frac{\dot{m}_a(L)}{\dot{m}_f(L)} = \frac{\rho_a(L)}{\rho_f(L)}$$

In order to take real gas effects into account, Siebers uses a generalized real gas equation of state in the form $p = Z \rho R T / M$, for both fuel and ambient gas. Combining this with Eq. (1), and assuming saturation at $x = L$, gives
\[
\frac{\dot{m}_f(L)}{\dot{m}_a(L)} = \frac{p^*}{p_a - p^*} \cdot \frac{M_f}{M_a} \cdot \frac{Z_f(T^*, p_a - p^*)}{Z_a(T^*, p_a - p^*)}
\]  
(2)

where \( Z_a \) and \( Z_f \) are the compressibility factors of the ambient gas and the vaporized fuel, respectively. (Later in this paper we discuss how this expression erroneously decouples the compressibility factors of fuel and ambient gas; however, here we merely present the original model.) \( M_f \) and \( M_a \) denote the molar masses of fuel and ambient gas. The saturation pressure \( p^* \) is a function of \( T^* \); for brevity’s sake this functional dependence is not written explicitly.

Applying the energy conservation law to the idealized spray results in
\[
\dot{m}_f(L) h_f(T_f, p_a) + \dot{m}_a(L) h_a(T_a, p_a) = \dot{m}_f(L) h_f(T^*) + \dot{m}_a(L) h_a(T^*, p_a - p^*)
\]  
(3)

where \( h_a, h_f, \) and \( h_f(T^*) \) represent the specific enthalpy of ambient gas and fuel (in both phases), with functional dependencies as indicated in Eq. (3).

Equations (2) and (3) are then combined to one nonlinear equation for the mass flow rate ratio \( B \):
\[
B = \frac{\dot{m}_f(L)}{\dot{m}_a(L)} = \frac{h_a(T_a, p_a) - h_a(T^*, p_a - p^*)}{h_f(T_f, p_a) - h_f(T^*, p_a)} = \frac{\frac{p^*}{p_a - p^*}}{M_f \cdot Z_f(T^*, p_a - p^*)} \cdot \frac{M_f \cdot Z_a(T^*, p_a - p^*)}{M_a \cdot Z_f(T^*, p_a - p^*)}
\]  
(4)

The unknown temperature \( T^* \) of the mixture at the liquid length can be found by iteratively solving Eq. (4). Once \( T^* \) is known, \( B \) follows from the same equation. Thus, \( B \) results as a function of \( T_a, T_f \), and \( p_a, \) together with appropriate physical property relations for fuel and ambient gas. The latter are determined in this work using a combination of empirically based correlations (DIPPR, 2009) and corresponding states estimation methods (Poling et al., 2001). Details are provided by Kurvers (2009).

In an earlier paper, Naber and Siebers (1996) showed that the conservation of fuel mass and total momentum results (within the same idealized spray model of Fig. 1) in the relation
\[
\frac{\dot{m}_a(x)}{\dot{m}_f(x)} = \sqrt{1 + 16\frac{x^2}{x^+} - 1} \over 2
\]  
(5)

where \( \bar{x} = x / x^+ \) and the length scale \( x^+ \) is given by
\[
x^+ = \frac{d_e}{a \tan(\theta/2)} \sqrt{\frac{\rho_f}{\rho_a}}
\]  
(6)

In this definition, the real spray angle \( \theta \) is introduced, which is related to the idealized angle \( \alpha \) by \( \tan(\alpha/2) = a \tan(\theta/2) \), where \( a \) is a constant with value 0.66, which corrects for the idealized spray shape used in the model. Experimental cone angle data are correlated well for vaporizing sprays by (Siebers, 1999)
\[
\tan(\theta/2) = c \left( \frac{\rho_a}{\rho_f} \right)^{0.19} - 0.0043 \sqrt{\frac{\rho_f}{\rho_a}}
\]  
(7)

where \( c \) is another constant, with value 0.26. Furthermore, \( d_e \) in Eq. (6) is the effective nozzle diameter \( d_e = d \sqrt{C_a} \), where \( d \) is the physical diameter of the orifice and \( C_a \) its coefficient of area contraction.

By applying Eq. (5) at \( x = L \) and using the definition of \( B \), one finds
\[
L = x^+ \bar{x}_L = 0.25 x^+ \sqrt{\left( \frac{2}{B} + 1 \right)^2 - 1}
\]  
(8)

Arguing that the theoretical factor 0.25 cannot be expected to give accurate results in view of the underlying severe simplifications, Siebers replaces it by an empirical constant \( b \) of value 0.41. Inserting (6) finally results in
\[
L = \frac{b}{a} \sqrt{\frac{\rho_f}{\rho_a}} \sqrt{C_a d} \left[ \frac{2}{B(T_a, p_a, T_f)} + 1 \right] \left( 1 - \frac{1}{B(T_a, p_a, T_f)} \right) \over 2
\]  
(9)

\[2.2\text{ Versaevel, Motte, and Wieser Model}\]

The other model considered in this study is the model by Versaevel et al. (2000), for brevity further denoted as the “Versaevel model”. These authors primarily used their model as a convenient means to introduce mass, momentum, and energy source terms in computational fluid dynamics (CFD) computations. This idea had been introduced by Wan and Peters (1997) based on droplet-limited vaporization. Abraham and Magi (1999) took a similar approach, assuming mixing-limited vaporization, not in the last place to prevent the notorious grid convergence problems with droplet-based spray models.

In essence, the Versaevel model is an extension of the Siebers model. Reconsidering Fig. 1, the major difference is that thermodynamic equilibrium is now assumed at every axial position \( x \) in the spray, from the orifice exit up to the liquid length. As a result, this model gives more insight in the spray formation upstream of the liquid length. This implies that more parameters appear, the most important one being the void fraction \( m \) upstream of \( x = L \). It also means that the conservation equations are solved at every axial position \( x \). Moreover, these are now fully coupled (from the previous section, recall that Eq. (5) was

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derived from fuel mass and overall momentum conservation, and applied separately from energy conservation. An explicit liquid length expression, analogous to Eq. (9) for the Siebers model, is not provided in the original publication (Versavel et al., 2000). Instead, in order to find the liquid length, the mass, momentum, and energy conservation laws are solved iteratively at every axial position in the spray. The liquid length is then given by the position \( x \) where \( m = 1 \).

Fuel mass conservation is expressed as

\[
\rho_f a_0 A v f_0 = \rho_f (1 - m) A v + Y_{fg} \rho_g m A v \tag{10}\]

where \( v \) is the axial velocity, again assumed uniform over the cross section of the spray with surface area \( A \). Introducing the mass flow rate ratio \( \Delta \), equivalent to \( 1/B \) in the Siebers model, this can also be written as

\[
\Delta = \frac{\dot{m}_a}{\dot{m}_{f0}} = \frac{m(1 - Y_{fg}) \rho_g}{\rho_f (1 - m) + m Y_{fg} \rho_g} \tag{11}\]

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. The subscript 0 denotes the nozzle exit. Other notations (as well as some others to come) have the same meaning as in the previous section.

Total momentum conservation can be written as

\[
\rho_f a_0 A v_f^2 = \rho_f (1 - m) A v^2 + \rho_g m A v^2 \tag{12}\]

Rewriting this in a similar fashion gives

\[
\Delta^2 = \frac{\rho_f a_0 A v_f^2}{\rho_f a_0 A v_f^2} = \frac{A m^2 (1 - Y_{fg})^2 \rho_g^2}{\rho_f (1 - m) \rho_f + m \rho_g} \tag{13}\]

The surface area ratio \( A/A_0 \) is fully determined by geometry (see Appendix). For each position \( x \), its value equals \( 1 + (2 x/d_e) \tan(\theta/2) \), with \( d_e \) as before. Versavel et al. use the same spray angle correlation (7) from Siebers (1999).

The law of energy conservation in this spray framework reads

\[
\dot{m}_{f0} h_f(T_f) + \dot{m}_a h_a(T_a) = \rho_f (1 - m) A v h_f(T) + Y_{fg} \rho_g m A v h_f(T) + \dot{m}_a h_a(T) \tag{14}\]

This equation can be rewritten in terms of specific heats, giving

\[
\Delta \int_T^{T_a} c_{pa}(s) ds = \left( \frac{Y_{fg} \Delta}{1 - Y_{fg}} - 1 \right) L_v(T) + L_v(T_f) + \int_T^{T_f} c_{pf g}(s) ds \tag{15}\]

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

The three basic conservation laws (11), (13), and (15) contain the unknowns \( \Delta, m, \rho_g, Y_{fg} \), and \( T \). Hence, two additional equations are needed. Upstream of (and up to) the liquid length, assumption of thermodynamic equilibrium states that the fuel partial pressure equals the fuel-saturated vapor pressure: \( X_{fg} = p^n/p_a \), where \( X_{fg} \) is the saturated fuel molar fraction (the notation used here is in accordance with conventions in combustion literature). Converting it into a mass fraction gives

\[
Y_{fg} = \frac{1}{\left( \frac{p_a}{p(T)} - 1 \right) \frac{M_f}{M_a} + 1} \tag{16}\]

Again assuming uniform pressure, \( \rho_g \) can be linked to \( T \) and \( Y_{fg} \) via

\[
\rho_g = \rho_a \frac{T_a}{T} \frac{1}{Y_{fg} \frac{M_f}{M_a} + [1 - Y_{fg}]} \tag{17}\]

Using the three nonlinear conservation equations (11), (13), and (15), and aided by Eqs. (16) and (17), the unknowns \( T, \Delta, \) and \( m \) can be found with a standard Newton-Raphson method.

In the above equations (as in the original paper) real gas effects are explicitly neglected. In the next section we show how real gas effects can be properly included in both the Siebers and Versavel models.

### 2.3 Real Gas Effects

Siebers’ original model takes into account real gas effects via the compressibility factors in Eq. (4). However, the implicit decoupling of fuel and ambient gas at the liquid length position cannot be justified. Since the molecules of ambient gas and fuel interact, the mixture should be considered as one medium. We now show how this can be done.

Since Eq. (1) directly results from mass conservation, it is also valid in a real gas context. Most generally we can write

\[
\frac{\rho_f(L)}{\rho_a(L)} = \frac{Y_{fg} \rho_g}{(1 - Y_{fg}) \rho_g} \frac{Y_{fg}}{(1 - Y_{fg})} = \frac{X_{fg} M_f}{(1 - X_{fg}) M_a} \tag{18}\]

which implies that the total mixture density \( \rho_g \) drops out of the equation. What remains to be determined is the saturated mole fraction \( X_{fg} \).
For ideal gases we have \( X_{fg} = p^*/p_a \). At higher densities, i.e., for real gases, \( X_{fg} \) can be computed from a flash calculation using an appropriate equation of state. In this work we have used the Peng-Robinson equation (Reid et al., 1987), which has a well-proven accuracy for high-pressure, nonpolar systems (relevant to diesel sprays). The fuel-ambient gas system is modeled as a two-component (binary) mixture, i.e., the different components of ambient gas are lumped. These components are nitrogen, oxygen, water vapor, carbon dioxide, and argon, depending on actual conditions (either in engines or in dedicated experiments, cf. Siebers, 1998).

In a binary flash calculation, the equilibrium conditions can be written as

\[
X_{fg} \Phi_g(p_a, T^*, X_{fg}, X_{ag}) = X_f \Phi_f(p_a, T^*, X_{ff}, X_{af}) \tag{19}
\]

\[
X_{ag} \Phi_a(p_a, T^*, X_{fg}, X_{ag}) = X_{al} \Phi_l(p_a, T^*, X_{fl}, X_{al}) \tag{20}
\]

The gas and liquid phase fugacity coefficients \( \Phi_g, \Phi_l \) can be derived from the equation of state (Reid et al., 1987). These coefficients depend on the molar fractions \( X_i \) of both components. For a binary system, the fractions of both sum up to unity in both phases, so that the two equilibrium conditions above, for given pressure and temperature, uniquely determine all the molar fractions involved. Notice that this only holds true for binary mixtures; with more components, the equilibrium composition becomes dependent on the input composition. Details of the implementation are described by Kurvers (2009).

To appreciate the magnitude of real gas effects on the equilibrium composition, it is advantageous (Luijten and Van Dongen, 1999) to introduce the enhancement factor \( f_e \) according to

\[
f_e = \frac{X_{fg} p_a}{p^*} \tag{21}
\]

Being defined as the ratio of saturated partial vapor pressure in a mixture over the saturated vapor pressure of the pure fuel, \( f_e \) is a direct measure of the deviation from ideal gas behavior. It contains several contributions: the effect of pressure on liquid chemical potential (Poynting effect), possible dissolution of the ambient gas into the liquid, and nonideality of the liquid phase and of both the saturated pure vapor and the high-pressure gas-vapor mixture (Prausnitz et al., 1986).

To illustrate the magnitude of the effect, Fig. 2 shows the enhancement factor as a function of pressure for a binary mixture of \( n \)-hexadecane and nitrogen. Obviously, \( f_e \) is unity for low pressure, independent of the temperature. Shown are temperatures around 500 K, which is a typical value of \( T^* \) for ambient gas temperatures around 800 K. With increasing pressure, the mixture deviates more and more from ideal gas behavior. At constant pressure, the enhancement factor decreases with temperature. Combining these observations, the conclusion is that the enhancement effect is largest at high pressure and low temperature, as expected.

For a given binary mixture, the enhancement factor can be correlated as a function of pressure and temperature in a preprocessing step, which removes the need to do flash calculations within the main routine of a spray model. For this purpose, it is advantageous to rewrite Eq. (18) using Eq. (21) as

\[
\frac{\rho_f(L)}{\rho_a(L)} = \frac{f_e p^* M_f}{(p_a - f_e p^*) M_a} \tag{22}
\]

The right-hand side of Eq. (22) replaces that of Eq. (4) in the original Siebers model, resulting in

\[
B = \frac{\dot{m}_f(L)}{\dot{m}_a(L)} = \frac{h_f(T_a, p_a) - h_g(T^*, p_a, X_{fg})}{h_g(T^*, p_a, X_{fg}) - h_f(T_f, p_a)} = \frac{f_e p^* M_f}{(p_a - f_e p^*) M_a} \tag{23}
\]

Effectively, the ratio of compressibility factors in Eq. (4) is replaced by the appearance of the enhancement factor in front of \( p^* \). Furthermore, it is to be noted that the enthalpy term \( h_g \) implicitly contains \( B \) [i.e., via the mixture composition; it can be shown that \( X_{fg} = (1 + B^{-1} M_f/M_a)^{-1} \)]. However, since Eq. (4) has to be solved numerically anyway, this is not a crucial complication.
Notice that the middle member of Eq. (23) has also changed with respect to Eq. (4). This is related to the effect of high pressure on enthalpy. For the sake of brevity, and since the resulting effect on liquid length turns out to be very small indeed (see Section 3), we only briefly describe the procedure to evaluate this effect. For details, the reader is referred to Kurvers (2009), which can be sent by the author upon request.

As stated before, the ambient gas and fuel vapor can no longer be decoupled in a real gas context. Taking this into account in the energy balance, the enthalpy of the mixture at the liquid length appears in the above equation, rather than those of the pure components. The mixture enthalpy \( h_g(T^*, p_a, X_{fg}) \) can be evaluated using so-called departure functions. Again, these can be derived from the Peng-Robinson equation of state (Reid et al., 1987).

Figure 3 presents the effect of pressure on all three enthalpy terms in Eq. (23). In addition, the enthalpy of the pure vapor is indicated for reference. Even at the pressure of 100 bar shown, the difference between ideal gas and real gas enthalpy is relatively small for all components. Therefore, it can be anticipated that the resulting effects on liquid length will be modest, since the effect of varying temperature is much larger than the pressure effect.

The derivation of the Siebers model after Eq. (4) in Section 2.1 does not change when including real gas effects. Specifically, we have checked that the derivation of Eq. (5) does not rely on any ideal gas assumptions.

In the Versaevel model, the enhancement factor formulation can also be used. Going back to its derivation, it can be seen that the basic conservation laws do not change. However, Eq. (16) turns into

\[
Y_{fg} = \frac{1}{\frac{p_a}{T_{p_a} p_a} - 1} \frac{M_e}{M_f} + 1
\]

since the first term in brackets effectively equals \( 1/X_{fg} \). As before, values of the enhancement factor are obtained from binary flash calculations, which can be done in a preprocessing step for a given mixture.

In the Versaevel model a second adaptation has to be made to include real gas effects. Equation (17) was derived using the ideal gas law \( (\rho = pM/RT) \) both for the gas mixture and ambient air. However, in a real gas context a generalized equation of state must be used \( (\rho = pM/RTZ) \). Applying this both for the ambient gas and for the gas-vapor mixture, Eq. (17) turns into

\[
p_g = p_a \frac{Z_a(p_a, T_a)}{Z_g(p_a, T_a, X_{fg})} \frac{T_a}{T} \frac{1}{Y_{fg} \frac{M_e}{M_f} + [1-Y_{fg}]}
\]

where \( Z_a \) is the compressibility factor of the ambient gas and \( Z_g \) that of the saturated gas-vapor mixture. Both can be calculated from the Peng-Robinson equation of state in combination with Van der Waals mixing rules (Reid et al., 1987). The compressibility factor of the ambient gas is constant for given ambient conditions. However, since the compressibility factor of the mixture depends on (changing) composition and temperature, it depends on axial position (recall that the Versaevel model is solved for every axial position \( z \)). This means that \( Z_g \) necessarily becomes part of the iterative solver routine.

Anticipating the results of the Siebers model in the next section, which show that the pressure effect on enthalpy has a very small effect on liquid length, the latter is not considered in the Versaevel model. Accordingly, Eqs. (14) and (15) are left unchanged.

3. RESULTS AND DISCUSSION

The main goal of this study is to assess the influence of real gas effects on both the Siebers and Versaevel liquid length predictions. In this section we first compare liquid length predictions from different versions of the Siebers model. Subsequently, liquid lengths resulting from the original and real gas versions of the Versaevel model are compared. Model results are also evaluated versus experimental liquid length data of \( n \)-hexadecane from Sandia National Laboratories (Pickett, 2007) and of \( n \)-dodecane from Verhoeven et al. (1998). In these comparisons, relevant parameters (such as nozzle diameters and area con-
traction coefficients, and fuel and ambient gas conditions) are taken from the original sources. Finally, differences between the Siebers and Versaevel models are evaluated and discussed in Section 3.3.

### 3.1 Real Gas Effects in Siebers’ Model

To assess the impact of real gas effects in the Siebers model, four versions of it are compared. The original model makes use of compressibility factors to include real gas effects. As was pointed out before, this approach is physically not fully correct. To assess the influence of these factors, a second model without any real gas effects is used for comparison. In a third variant, the impact of high pressure on the phase equilibrium is included using the enhancement factor, as explained previously. The fourth variant includes both the enhancement effect and the pressure effect on enthalpy.

Figure 4 shows the results of these four models as a function of ambient temperature and at constant ambient pressures of 10 and 100 bar. The fuel is \( n \)-hexadecane (\( C_{16}H_{34} \)), which has a boiling point in the diesel range and, therefore, is a widely used surrogate fuel for diesel evaporation.

From Fig. 4a we can deduce that all four models predict very similar liquid lengths at 10 bar. For all models \( L \) decreases with increasing ambient temperature. The model without real gas effects results in the longest values, whereas the “full real gas” model (with enhancement factor and real gas enthalpy) results in the shortest liquid lengths. The other two models are in between.

Figure 4b shows similar data at 100 bar, which is at the very upper end of the range of realistic in-cylinder pressures in current diesel engines at the start of injection. At this pressure, differences in liquid length predictions between the four models become significant. All trends remain the same, but absolute values of the liquid length are much shorter than at 10 bar.

Zooming in on the differences between models at 100 bar, Fig. 5 shows the deviation of each model with respect to the full real gas model. As expected, the difference between the models with ideal and real gas enthalpy is very small, less than 4%, which is roughly 1 mm at a liquid length of 25 mm (see Fig. 4b). This is smaller than the typical accuracy of experimental data (the reported 1σ standard deviation of the Sandia data is ±2%; Siebers, 1998). Hence, we can conclude that the influence of real gas effects on enthalpy can be neglected. In the remaining sections of this paper, ideal gas enthalpy is therefore used in all models.

Figure 5 also demonstrates that the original Siebers model results in shorter liquid lengths than the ideal gas one but longer than the full real gas model. Thus, although Siebers’ approach using compressibility factors acts in the right direction, it underestimates the impact of real gas effects on liquid length.

In Fig. 6a the liquid lengths computed with the original and real gas Siebers models are shown, combined with experimental data from Pickett (2007). The latter data set was used to tune the constant \( b \) in the original model [see Eq. (9)]. The closed symbols represent experimental data, while the line styles (combined with open symbols) represent the different models. Figure 6b shows the relative error of the models with respect to the data. For clarity, this is only done for three densities (the outer two and middle values).

![Figure 4](image_url) **FIG. 4:** Liquid length model results as a function of ambient temperature for \( n \)-hexadecane in nitrogen. (a) 10 bar and (b) 100 bar.
At low ambient densities the difference between the models is negligible, in accordance with expectation. At low ambient density and low temperature, the predictive capability of both models is very poor. Most probably, this can be attributed to violation of the mixing-limited assumption at these conditions. This hypothesis is supported by the observation that the error gets smaller with increasing temperature, while staying at the same low density. Obviously, inclusion of real gas effects cannot “repair” this model deficiency at low density.

Figure 6 also reveals that the original and real gas Siebers model differ most at an ambient density of 58.5 kg/m$^3$. Looking only at the two highest densities in Fig. 6b (relevant to in-cylinder diesel engine conditions), it is observed that the overall spread in the errors is smaller for the real gas model. This indicates a better capability of the full real gas model to predict trends. Closer inspection reveals that this is caused by larger real gas corrections at lower temperatures versus smaller corrections at higher temperatures.

Overall, especially at high ambient density and low ambient temperature, the real gas model has an improved predictive capability over the original model, which might be further enhanced by adjusting the constant $b$ in Eq. (9). To do so, however, would require careful reconsideration of the whole data base (with more fuels and experimental conditions). Such an attempt is beyond the scope of the present paper.

### 3.2 Real Gas Effects in Versaevel’s Model

In this section, results of the Versaevel model are compared to experimental liquid length data. In contrast to the Siebers model, the Versaevel model was originally compared to data from Verhoeven et al (1998) for $n$-dodecane. Therefore, model results are first compared with the latter data. However, the model constants were not explicitly optimized for this data set (see Section 3.3).

In Fig. 7 liquid length results of the original and real gas Versaevel model are compared with data for $n$-dodecane ($C_{12}H_{26}$) at a temperature of 800 K. For comparison, liquid length results of the real gas Siebers model are plotted as well. Liquid lengths computed with the real gas Siebers model are in general a few millimeters longer than those from both Versaevel model variants. At first this seems strange, since both models are derived using basically the same assumptions and conservation laws. A closer discussion of this observation is postponed to the next section.
FIG. 7: Liquid length as a function of ambient density at 800 K for \( n\)-dodecane. Experimental results of Verhoeven et al. (1998).

At an ambient density of 12 kg/m\(^3\), the original Versaevel model appears closer to the experimental data than the real gas version. At higher ambient densities (25 and 30 kg/m\(^3\)), the real gas model variant is closer to the data. It is tempting to conclude that this is caused by real gas effects becoming more important with increasing ambient density; however, one should keep in mind that both models contain at least one empirical constant, the adjustment of which causes all models to collectively shift up and down. Therefore, based on this limited amount of data, no firm conclusion can be drawn from Fig. 7 with respect to the predictive capability of either of the models. Doing so requires a larger database which enables study of more trends.

Therefore, it is interesting to see what the predictive capability of both real gas models is with respect to Sandia data. Figure 8a displays the real gas Siebers and Versaevel model, denoted by the different line styles with open symbols. It also includes experimental data from Sandia (Pickett, 2007), represented by closed symbols. As expected from Fig. 6, again the liquid lengths computed with the real gas Siebers model are close to the experimental data, at least for the higher densities. Predictions by the Versaevel model, however, are significantly shorter than the real gas Siebers results. Thus, the Versaevel model underpredicts the Sandia data.

This observation is magnified in Fig. 8b, showing the deviations of both models with respect to the Sandia data. Again, only the outer two and middle density are shown to prevent cluttering of the figure. The real gas Versaevel model underpredicts the data at almost every condition. At the lowest temperature (700 K) the deviation is relatively small (within 20%). For higher temperatures, especially 1300 K, this increases to approximately 35%, regardless of ambient density. Overall, it can be concluded that the predictive capability of the Versaevel model with respect to the Sandia data is worse than that of the Siebers model. These findings will now be further discussed.

3.3 Discussion

To explain the differences between the Versaevel and Siebers models, we look at the explicit liquid length equations of both models. For the Versaevel model, the original paper does not provide a closed expression. In the Ap-
pendix we show how such an expression can be derived. To facilitate reading, both expressions are reproduced below. The Siebers equation is

\[
L = \frac{b}{a} \sqrt{\frac{\rho f_0}{\rho a}} \sqrt{C_0 d} \tan(\theta/2) \sqrt{\left(\frac{2}{B} + 1\right)^2 - 1}
\]  

(26)

whereas the Versaevel model can be cast in the form

\[
L = \frac{1}{4a} \sqrt{\frac{\rho f_0}{\rho_a(L)}} \sqrt{C_0 d} \tan(\theta/2) \sqrt{\left(\frac{2}{B} + 1\right)^2 - 1} - \frac{1}{2a \tan(\theta/2)}
\]  

(27)

Looking at both expressions, four differences appear. The most obvious one is that Eq. (27) contains an additional term. Physically, it takes into account that the actual starting point of the “spray triangle” of Fig. 1 is located slightly inside the nozzle hole. In the Siebers model, this term is neglected (actually, it is omitted in the derivation of the penetration scaling law, see Naber and Siebers, 1996).

The magnitude of the additional term is about 1–2 mm in liquid length at typical in-cylinder conditions. The first term is usually on the order of 10–100 mm. Therefore, the additional term is only significant at the lowest values of \(L\), that is, at the highest temperature and density. Since the underprediction in Fig. 8b occurs for all densities, we can conclude that the influence of the nozzle area correction can be neglected.

A second difference between both models, “hidden” in the above expressions, are possible differences in the values of \(B\). In terms of the Versaevel model, \(B\) corresponds to \(1/\Delta\), both representing the fuel-air mass ratio. To assess possible differences in \(B\), Fig. 9 provides values of this parameter for all models involved. By comparing Figs. 9a and 9b, it is apparent that the \(B\) values of the Siebers model without \(Z\) (i.e., without real gas effects) correspond very well to those of the original Versaevel model. Likewise, the real gas values of \(B\) correspond very well to those of the real gas Versaevel model.

A closer analysis of Eq. (14), inserting \(m = 1\) at \(x = L\), reveals that it is actually equivalent to Eq. (3), within the ideal gas enthalpy assumption. Hence, it appears that the determination of \(B\) (and therefore of \(T^s\)) is the same in both models. This is confirmed by Fig. 10, providing saturation temperatures \(T^s\) for all models involved. Indeed, the original Versaevel model values fall on top of those for Siebers without \(Z\) (both ideal gas). The
real gas versions of both models also coincide. The original Siebers model (with \( Z \)) is in between, as expected.

One should be aware that the above observations do not imply that the fuel-air ratio and temperature fields are the same in both models. Although the values at the liquid length \( L \) coincide, \( L \) itself differs between the models as a result of fuel mass and momentum considerations (resulting in different densities in the equations, see below). Since the Versaevel model results in shorter liquid lengths, the fuel-air ratio falls off faster with downstream distance, and temperature increases faster than in the Siebers model. This, in turn, must be caused by the effect that evaporation has on fuel mass and momentum conservation. The change in the fuel-air ratio field is important when the model is used, as intended by its authors, to represent source terms in CFD.

The third difference between Eqs. (26) and (27) is the density ratio under the square root sign. In the Siebers equation \( \rho_a \) is evaluated at ambient temperature \( T_a \), without fuel vapor. In the Versaevel equation the ambient gas (partial) density is evaluated at the liquid length, so at temperature \( T^a \) and the prevailing (saturated) vapor fraction. These are competing effects; the lower temperature \( (T^a \text{ versus } T_a) \) tends to increase \( \rho_a(L) \), whereas the presence of fuel vapor decreases it. Using an ideal gas approach to estimate density, it can be proven that the factor between the Siebers and Versaevel models due to this density ratio amounts to (with \( f_c \) set to unity for the ideal gas model)

\[
\sqrt{\rho_a} = \sqrt{\frac{T^a}{T_a(1 - X_{f,g})}} = \sqrt{\frac{T^a}{T_a(1 - f_{evap}^s/p_a)}}
\] (28)

Figure 11 shows this correction factor for the ideal and real gas Versaevel models. By comparison with Fig. 8, it can be concluded that this factor accounts for the larger part of the differences between the Siebers and Versaevel model results. Again, since the density ratio in both models results from only fuel mass and momentum conservation, the conclusion is that upstream evaporation significantly affects fuel mass and momentum conservation.

A final difference between both models is the factor \( 1/4 \) in Eq. (27), which replaces parameter \( b \) in Eq. (26). As indicated in Section 2, Siebers states that the theoretical value of \( b \) would be 0.25 but replaces it by 0.41 to improve agreement of his scaling law with experiment. Versaevel, on the other hand, fits the product \( (a \cdot c) = 0.104 \) to obtain optimal agreement with experiments. Since he uses the same cone angle correlation, \( c = 0.26 \), so the effective \( a \) value is 0.40. Hence, the effective “\( b/a \)” value in the Versaevel model is 0.625. This can be compared to \( b/a = 0.621 \) for the Siebers model. Effectively, we can conclude (as Versaevel et al. do) that the difference is not in the fit parameters.

This does not mean that the fit parameters are optimal. As we have seen above, the enhancement effect leads to smaller liquid length predictions; to restore agreement with data, the value of \( b \) would need to increase. This is in correspondence with more detailed spray models: realistic profiles show a peak vapor fraction on the spray axis, decaying to zero at the spray edges. According to Desantes et al. (2007), the on-axis vapor fraction is twice the cross-sectional average; as a result, any cross-sectional average model would give too low predictions of \( L \), since the on-axis fuel vapor fraction determines the maximum liquid length in experiments. In the model by Desantes et al., the liquid length is proportional to \( 1/Y_{f,evap} \), so the above effect would lead to a factor of 2 correction of a cross-sectional average model. This would imply a value of \( b = 0.50 \) in the Siebers model, which is about 20% higher than the value Siebers uses (in other words, the “theoretical value” 0.25 does not take into account this radial correction). This would lead to an upward shift of all points in Fig. 8b, in favor of the Versaevel model.

In the models discussed here, the liquid length is proportional to \( \sqrt{B + 1/B} \), as can be shown by rewriting Eq. (26). Since \( B = Y_f/(1 - Y_f) \), \( L \) is proportional to \( \sqrt{1 - Y_f}/Y_f \). Due to this functional dependence, a factor of 2 in \( Y_f \) (due to cross-sectional averaging) will give a correction of \( L \) that varies with conditions. Such a temperature-dependent correction might be responsible for the remaining temperature trend in the Versaevel data in Fig. 8b.
Finally, in a later paper (Siebers et al., 2002) the constant $C_a$ was adjusted to 0.75, based on new measurements of the area contraction coefficient $C_a$. Yet, because the new values for $C_a$ were not published, we decided to keep using the old $C_a$ values with $a = 0.66$. This does not affect liquid length, since the ratio $\sqrt{C_a}/a$ appearing in the equations should be the same for both combinations. However, it does indicate that for prediction of absolute numbers, it is key to have the right set of constants available for the injector of interest.

Summarizing, we can conclude that the predictive capability of the Siebers model (at least with regard to Sandia data) is better than that of the Versaevel model. This might still be due to a cancelation of underestimated real gas effects and a too low model constant $b$. Inclusion of real gas effects makes the model predictions at high densities more consistent. The Versaevel model seems physically more correct, since it captures better the physics of the vaporizing spray. Careful analysis of the differences between both models has shown that the difference in ambient (partial) density in the liquid length equation is directly responsible for most of the difference between the models.

Consequently, a correction factor based on Eq. (28) could be implemented to “translate” the Siebers model into the Versaevel model, accounting for the effect of evaporation on fuel mass and momentum conservation. The main argument against this would be that the errors in Fig. 8b show a temperature trend for the Versaevel model. Including a correction as suggested above would give a temperature trend in the errors for the Siebers model as well.

It was conjectured that this remaining temperature trend is due to cross-sectional averaging over the spray. Taking into account realistic radial profiles leads to both a larger constant in the $L$ equations and to a correction that depends on conditions. Therefore, this effect could be responsible for both the remaining temperature trend and the remaining absolute error in Fig. 8b. Therefore, it seems that the only way to further improve mixing-limited models is to include the radial direction, as Desantes et al. (2007) have done. Their approach allows adjustable model constants to be avoided altogether.

4. CONCLUSIONS

Critical evaluation of two existing mixing-limited spray vaporization models, by Siebers (1999) and Versaevel et al. (2000), has shown that in these models real gas effects were implemented incorrectly and not at all, respectively. Going back to first principles, both models were derived again using the enhancement factor to include the effect of an increasing saturated vapor pressure with ambient gas pressure. Values of enhancement factors were obtained from flash calculations using the Peng-Robinson equation of state. By doing so, the account for real gas effects in the Siebers model was improved, whereas inclusion of real gas effects in the Versaevel model was done for the first time.

Both original models use ideal gas enthalpy in their equations. The Siebers model was used to assess the influence of real gas enthalpy on liquid length predictions. Departure functions were used to account for pressure effects on enthalpy, which were evaluated from the Peng-Robinson equation of state. Comparing model predictions at 100 bar, using ideal and real gas enthalpy, it was concluded that the influence of nonideal enthalpy on liquid length can be neglected.

Comparing liquid lengths of the Siebers model with data from Pickett (2007) has shown that inclusion of real gas effects improves its predictive capability at high densities. At low densities the liquid length prediction of both original and real gas models is very poor, probably because the vaporization of fuel is no longer controlled by the mixing rate of fuel and air. At these conditions droplet-limited vaporization models should be considered instead.

An improvement in predictive capability at high density by including real gas effects was also observed for the Versaevel model by comparing original and real gas model results with experimental data. However, the data set on which this conclusion is based might be too small to be significant.

In comparing results of the Siebers and Versaevel models it was seen that they give different predictions, in spite of using almost the same assumptions and conservation laws. To analyze this, an explicit liquid length equation for the Versaevel model was derived. Comparing it with the Siebers equation revealed that the main difference is in the evaluation of ambient (partial) air density in the liquid length expression. The analysis also showed that the fuel-air ratio field is significantly influenced by real gas behavior. This is important, for example, when mixing-limited models are used to represent source terms in CFD modeling. Another conclusion from the comparison is that the effect of evaporation on fuel mass and momentum conservation is significant.

A correction factor was derived that “translates” the Siebers model into the Versaevel expression. The latter is believed to more consistently capture the physics of
a vaporizing spray. However, prediction of temperature trends observed in the data did not directly benefit from this correction, for the limited data set considered in this work. It was conjectured that both the remaining temperature trend and the absolute level in the errors of the Versaevel model could be due to the cross-sectional averaging approach. Including variations over the radial direction in the model can also avoid the need for using adjustable model constants. Yet, for accurate quantitative predictions, this does not take away the need for using accurate values for experimental parameters such as nozzle diameters and discharge coefficients.

APPENDIX. EXPLICIT LIQUID LENGTH EQUATION FOR VERSAEVEL’S MODEL

In order to compare the Siebers and Versaevel models on a more fundamental level, an explicit liquid length equation for the latter will be derived. To do so, reconsider the momentum balance (12). For the aim of deriving an expression for \( L \), our interest can be confined to the liquid length only. This means that the void fraction \( m \) can be set equal to unity, which leads to

\[
\rho_f A_0 v_f^2 = \rho_g(L) A(L) v(L)^2 \tag{A.1}
\]

Since at the liquid length no liquid fuel is left, the total density of the gas phase is \( \rho_g(L) = \rho_f(L) + \rho_a(L) \). Equation (A.1) can then be written as

\[
\rho_f A_0 v_f^2 = \rho_f(L) A(L) v(L)^2 + \rho_a(L) A(L) v(L)^2 \tag{A.2}
\]

Notice that \( \rho_f(L) \) here denotes the mass density of fuel vapor at \( x = L \). Using the familiar expressions \( \dot{m}_f = v_f \rho_f A_0 \) and \( \dot{m}_a(L) = v(L) \rho_a(L) A(L) \) to eliminate \( v_f \) and \( v(L) \), the momentum balance becomes

\[
\frac{\dot{m}_f^2}{\dot{m}_a(L)^2} = \frac{\rho_f(L)}{\rho_a(L)^2} \frac{\dot{m}_a(L)^2}{A(L)} + \frac{\dot{m}_a(L)^2}{\rho_a(L)^2 A(L)} \tag{A.3}
\]

or, after rearrangement,

\[
\frac{\dot{m}_f^2}{\dot{m}_a(L)^2} = \frac{\rho_f(L)}{\rho_a(L)^2} \frac{A_0}{A(L)} \left[ \frac{\rho_f(L)}{\dot{m}_a(L)^2} \frac{A_0}{A(L)} \left( \frac{\rho_f(L)}{\rho_a(L)} \frac{A_0}{A(L)} \right) + 1 \right] \tag{A.4}
\]

From Eq. (4) it appears that the left side of (A.4) equals \( B^2 \). Notice that the density ratio between right brackets also equals \( B \). Furthermore, the cross-sectional area at the liquid length is given by

\[
A(L) = \pi \left( \frac{d_e}{2} + L \tan(\alpha/2) \right)^2 \tag{A.5}
\]

The surface area of the nozzle exit is \( A_0 = (\pi/4)d_e^2 \). In these expressions \( d_e \) denotes the effective nozzle diameter and \( \alpha \) is the idealized spray angle from Fig. 1. Substituting these expressions into Eq. (A.4) gives

\[
B = \frac{\sqrt{\rho_A f}}{\sqrt{\rho_a(L)}} \frac{\frac{d_e}{2} + L \tan(\alpha/2)}{\sqrt{B + 1}} \tag{A.6}
\]

Using \( d_e = \sqrt{C_ad} \), where \( C_a \) represents the area contraction coefficient and \( d \) denotes the nominal diameter of the nozzle, Eq. (A.6) can be rewritten as

\[
L = \frac{1}{2} \sqrt{\frac{\rho_A f}{\rho_a(L)}} \frac{\sqrt{C_ad}}{\tan(\alpha/2)} \sqrt{B + 1} - \frac{1}{B} \frac{\sqrt{C_ad}}{\tan(\alpha/2)} \tag{A.7}
\]

Rearranging and using \( \tan(\alpha/2) = a \tan(\theta/2) \) finally gives

\[
L = \frac{1}{4a} \sqrt{\frac{\rho_A f}{\rho_a(L)}} \frac{\sqrt{C_ad}}{\tan(\theta/2)} \left( \frac{2}{B} + 1 \right) - \frac{1}{2a \tan(\theta/2)} \tag{A.8}
\]

In this way, Eq. (A.8) is written in a similar form as Siebers’ Eq. (9). Both expressions are compared and critically evaluated in Section 3.3.

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