ABSTRACT
Lowering diesel engine emission levels, while preserving performance, is the main demand in the development of current and future diesel engines. To fulfill it, the in-cylinder vaporization and combustion processes of the diesel spray must be well understood.

An important parameter in the vaporization process of a diesel spray is the maximal penetration distance of liquid fuel (i.e. the “liquid length”). So-called mixing-limited vaporization models assume that the vaporization rate of the fuel is limited by the mixing rate of fuel and ambient gas. Such models have been shown in the literature to accurately correlate liquid lengths for moderate to high in-cylinder densities, i.e. in the density range relevant to modern diesel engines.

Since in-cylinder pressures can reach high absolute levels, real gas effects should be considered in these models. Critical evaluation of the most commonly used mixing-limited vaporization model (Siebers, SAE 1999-01-0528) reveals that real gas effects are not implemented consistently, since compressibility factors of the fuel and ambient gas are decoupled.

In this work the Siebers model is adapted to properly include real gas effects, using saturated vapor fractions from equilibrium flash calculations based on the Peng-Robinson equation of state. Results of the original and revised models are compared to experimental liquid length data from Sandia National Laboratories for various fuels, densities and temperatures.

At relatively low ambient densities, the original and revised models give identical results, as expected. At higher densities, more relevant to current and future diesel engines, the difference becomes significant. Moreover, liquid lengths computed with the revised model are closer to experimental data, especially at the highest ambient pressures. It is concluded that the overall predictive capability of the Siebers model can be improved using the method to include real gas effects presented here.

INTRODUCTION
With the increasing need to meet stringent emission limits, knowledge of the internal processes in a direct injection diesel engine becomes increasingly indispensable. Vaporization of the liquid core of the fuel spray plays a key role in the diesel process. More specifically, understanding of the maximal penetration of liquid fuel into the cylinder (often referred to as the “liquid length”) is crucial to avoid wall-wetting, which can lead to unacceptable emission levels, especially with early injection strategies. The latter have received increasing attention with the advent of PCCI-like combustion concepts. The liquid length is also important to understand the general behavior of a combusting fuel spray. Since several regimes can occur, depending on the magnitude of both liquid length and flame lift-off length [1], it is crucial to measure, analyze and understand both.

Due to turbulence, the tip of the liquid fuel region in practice fluctuates around a mean location. Typically, this mean location (quasi-steady liquid length) is measured by illuminating the spray, recording the Mie scattering signal from liquid droplets, followed by averaging over many instantaneous images [2,3]. The liquid length is then determined from the intensity profile on the centerline of the spray, using a threshold either on intensity [2] or on its derivative [3]. Choosing such a threshold obviously introduces some arbitrariness to the experimental values of liquid length. Although the repeatability of the experimental data (quasi-steady values) discussed here is quite good (± 2% 16 according to Ref. [2]), their accuracy is hard to specify. As
a consequence, comparing trends in model results with data is more useful than comparing absolute values.

Sandia National Laboratories have an outstanding track record of different kinds of measurements in diesel sprays, which have been made available to the public [4]. From the same group of workers, also a specific class of scaling correlations has evolved, based on the assumption of an effectively one-dimensional spray (i.e. properties such as velocity and air-fuel ratio are assumed to be effectively uniform over each axial cross-section of the spray). Using this model framework, a correlation for spray penetration was first derived [5], followed by a scaling law for liquid length based on mixing-limited vaporization [6]. Later the model was extended to include properties relevant to combustion, such as equivalence ratio at flame lift-off length [1,7], overall oxygen ratio [8] and even ignition phenomena [9].

The liquid length scaling law of Siebers [6] was shown by its inventor to give quite accurate predictions of liquid length at conditions relevant to modern diesel engines. For a common compression ratio of 17, a realistic in-cylinder density at SoI would be between 18 (low load, no turbo charging) to 50 kg/m³ (turbo-charged heavy duty diesel at full load, but without EGR). Corresponding pressures, with a typical temperature at SoI of 900 K, are in the range of 45 to 130 bar. With EGR these values may be even higher.

At lower temperatures and/or densities, the predictive capability of mixing-limited vaporization models was shown to decrease [6]. More specifically, predicted liquid lengths become too large at low temperatures. One, seemingly obvious, explanation would be that the main assumption of the model breaks down at lower density and/or temperature: evaporation is no longer mixing-limited. Rather, local inter-phase transport (i.e., droplet evaporation) starts to become the limiting factor. However, at a closer glance, one would expect that results of such droplet-limited liquid length models would be larger than mixing-limited model results. If droplet evaporation forms an extra limiting step in vaporization (next to hot air entrainment), predicted liquid lengths are expected to go up when this effect is properly taken into account.

An alternative explanation of the partial model deficiency at low temperature could be the following. It is known that a high ambient pressure can have a pronounced effect on vapor-liquid equilibrium [10]. More specifically, the absolute maximum vapor content of a vapor-gas mixture increases with ambient gas pressure. Moreover, the effects that are causing this - mainly the non-ideality of the saturated, pressurized mixture - are bound to increase at lower temperatures. Along this line of reasoning, one may expect that fuel will evaporate more easily at high pressure and moderate temperature. Ignoring this effect would thus give too large liquid length predictions, which might explain the observations at lower temperatures. This conjecture has been at the basis of the present work.

In the next section we carefully reconsider the liquid length scaling law derivation by Siebers. We thereby incorporate real gas effects in a more strict and extended manner than he did in Ref. [6]. In the third section, results of our revised model will be compared to those of the original model, and to the experimental data [4] that it was based on. The paper ends by summing up its main conclusions.

**SIEBERS' SCALING LAW REVISITED**

In this section the derivation of the original scaling law by Siebers [6] is briefly revisited. We pinpoint the steps where real gas effects come into play, and explain how these can be properly accounted for.

A key parameter in Siebers' model is the ratio between the mass flow rates of fuel and air at the liquid length, denoted as B. Within the assumptions of the model, fuel and air are well mixed and have equal (and radially uniform) velocities. Therefore this mass flow ratio equals the ratio of partial densities:

\[ B = \frac{\dot{m}_f(L)}{\dot{m}_a(L)} = \frac{\rho_f(L)}{\rho_a(L)}. \]  

(1)

To take into account real gas effects, Siebers introduces the generalized equation of state \( \rho = \frac{pM}{ZR_0T} \) where \( p \) is pressure, \( T \) temperature, \( R_0 \) the universal gas constant, \( M \) a molar mass and \( Z \) a compressibility factor. Furthermore, assuming a saturation condition at the liquid length, the partial pressure of the fuel vapor is put equal to \( \rho_f \), and that of the ambient gas to \( \rho_a \). This results in the equation

\[ B = \frac{p_f}{p_a - p_f} \frac{M_f}{M_a} \frac{Z_f(T_s, p_a - p_f)}{Z_a(T_s, p_a)}, \]  

(2)

The appearance of the third factor on the right hand side is questionable, since it assumes that fuel and ambient gas do not interact within the spray. Obviously, since the concentrations of fuel and air are not too far apart, their molecular interactions need to be taken into account.

A better way to take into account the high pressure thermodynamics of the mixture is to realize that the partial density ratio in Eq. (1) is just equal to the ratio of mass fractions times the total density. Hence, total density cancels from the equation, leaving...
Here we have introduced $Y_f$, the mass fraction of fuel in the saturated fuel-ambient mixture. For brevity it was directly converted to the molar fraction $X_f$, which connects better to the thermodynamics of saturation.

For an ideal gas-vapor mixture, the saturated molar vapor fraction is equal to the saturated vapor pressure over the total pressure: $X_f = p_s / p_a$. However, for real gases this no longer holds; as indicated in the introduction, the partial saturated vapor pressure increases with total pressure. This effect can be straightforwardly computed using an appropriate equation of state. In this work we have used the Peng-Robinson equation \[11\]. Methods to obtain phase equilibrium data from it are extensively described, for instance, in Ref. \[12\]. To appreciate the magnitude of the effect, it is noted here that the saturated partial pressure can increase more than a factor two over its normal (pure vapor) value, for typical spray core conditions (around 500 K, and up to 100 bar).

For a binary mixture, i.e. when the fuel is modeled as a pure hydrocarbon and the ambient gas is modeled as one effective component by lumping its constituents, the equilibrium molar fractions are fully determined by temperature and pressure, hence $X_f = X_f(T_s, p_a)$. (Notice that this does not hold for mixtures with more components; in that case one or more “feed” fractions need to be specified in the flash calculation, in order to “close” the flash problem).

The next important step in Siebers' derivation is to determine the ratio $B$ again using energy conservation. Fuel and ambient gas enthalpies ($h_f$ and $h_a$, respectively) are again decoupled, resulting in

$$B = \frac{h_a(T_s, p_a) - h_a(T_s, p_f)}{h_f(T_s) - h_f(T_f, p_a)}.$$ \[4\]

Decoupling of fuel and ambient gas in this equation is only justified if the total enthalpy is additive. Strictly speaking, this is not the case: besides contributions from the individual components of the mixture, there can be an extra (positive or negative) contribution due to the interaction between components. This can be expressed using so-called departure functions \[11,12\].

Secondly, the use of different partial pressure levels in Eq. \(4\) is also questionable, since the vapor-ambient gas mixture as a whole is at a certain total pressure. Going back to basics, the energy conservation law can be written for the given situation (also for non-ideal mixtures) as

$$\dot{m}_a h_a(p_a, T_a) + \dot{m}_f h_f(p_a, T_f) = (\dot{m}_a + \dot{m}_f) h_g(p_a, T_s, X_f),$$ \[5\]

where $h_g$ now denotes the enthalpy of the mixture at the saturation condition (temperature $T_s$ and total pressure $p_a$). Notice that the fuel vapor fraction appears as a third parameter in $h_g$. Converting this to explicitize $B$, we get

$$B = \frac{h_a(T_s, p_a) - h_g(T_s, p_a, X_f)}{h_g(T_s, p_a, X_f) - h_f(T_f, p_a)}.$$ \[6\]

In implementing this equation, we have used departure functions \[12\] based on the Peng-Robinson equation \[11\]. Great care was taken of appropriate reference enthalpy states for both fuel and ambient gas (when this is omitted, one easily gets erroneous results!).

Figure 1 shows the enthalpy of the fuel (modeled here as n-hexadecane), ambient gas (with a composition corresponding to that of the typical experimental data from \[4\], used later in this paper: mole fractions are 0.8971 nitrogen, 0.0377 water and 0.0652 carbon dioxide) and the vapor-gas mixture as a function of pressure. It can be observed that, for all components, the difference between ideal and real enthalpy is minimal (i.e., much smaller than the effect of temperature), even at the relatively high pressure of 100 bar applied in Fig. 1. Therefore, it is expected that the influence on liquid length will indeed be negligible, as assumed by Siebers.

Overall, the non-linear equation for $B$, which is at the heart of Siebers' scaling law, becomes

$$B = \frac{h_a(T_s, p_a) - h_g(T_s, p_a, X_f)}{h_g(T_s, p_a, X_f) - h_f(T_f, p_a)} = \frac{X_f(T_s, p_a)}{1 - X_f(T_s, p_a)} \frac{M_f}{M_a}.$$ \[7\]

Obtaining the saturated fraction from equilibrium flash calculations, and using the appropriate enthalpy routines, both the equilibrium temperature $T_s$ and the ratio $B$ are obtained for real gas thermodynamic conditions.
We have carefully confirmed that other steps in the derivation of the original scaling law do not contain any assumptions on ideal gas behavior. The final expression for liquid length \( L \) is therefore not affected, except that \( B \) is determined differently. For completeness, the final liquid length equation is reproduced here:

\[
L = \frac{b}{a} \sqrt{\frac{\rho_f}{\rho_a} \tan(\alpha/2)} \left( \frac{2}{B} + 1 \right)^2 - 1.
\]  

(8)

In this equation, \( b \) is an empirical constant (with theoretical value 0.25, but set equal to 0.41 by Siebers to arrive at the best agreement with experimental data); \( a \) is the proportionality constant between the idealized spray angle \( \alpha \) and real spray angle \( \theta \); \( d_0 \) is the (nominal) nozzle diameter and \( C_a \) its coefficient of area contraction.

**RESULTS AND DISCUSSION**

In this section the liquid length results of the original and revised models are compared to experimental data [4] on which the original model was founded.

Figure 2 shows liquid length results of the original model and of the “full real gas model” described above, as a function of ambient temperature for n-hexadecane. The experimental data is represented by closed symbols.

At low densities (up to about 15 kg/m\(^3\)), the difference between the original and real gas model liquid lengths is very small. Obviously, real gas effects do not play a role at these conditions. However, for higher ambient densities, corresponding to the density range relevant to modern diesel engines (starting at about 18 kg/m\(^3\)), these do become important, leading to increasing differences in liquid length between the two models.

Furthermore, Fig. 2 shows that the predictive capability of the Siebers model increases with the inclusion of real gas effects, especially at high ambient density levels in the lower temperature range, where the full real gas model is now closer to experimental data than the original model.

At the lowest ambient density the prediction of liquid length is poor for both models. As indicated in the previous section, it is tempting to conclude that this observation is due to fuel vaporization no longer being controlled by mixing of fuel and air. However, as explained there, if this is the reason for the observed deviation one would expect any mixing-limited model to underpredict (instead of overpredict) liquid lengths. Moreover, as discussed earlier, it must be noted that the lowest densities in Fig. 2 are not very relevant to evaporation conditions in modern diesel engines.

Figures 3 and 4 show again the liquid lengths computed with the original and revised models versus temperature, but now experimental data of HMN (heptamethylnonane) and D2 (again from Ref. [4]) is taken, respectively. Since D2 is a standard diesel fuel, it consists of multiple components, which can at present not be used as input in the models. However, as shown by Siebers in Ref. [6], measured liquid lengths of D2 are very well correlated using n-heptadecane as
a fuel in the scaling law; therefore the latter is used in both models.

In both figures, again the difference between the models is small at the lowest density, as expected, while at the highest density the difference is much larger. With respect to the experimental data, Fig. 3 shows the same trend as Fig. 2. At the lowest ambient density, liquid length prediction is poor with both models, while at the (more relevant) higher ambient densities the revised model fits the data better. The same trend is seen in Fig. 4, although at the highest ambient density and lowest temperature, the revised model now underpredicts the liquid length. This may for a large part be caused by replacing D2 by n-heptadecane in the model. The heavier fraction of real diesel fuel may, especially at these low temperature conditions, dominate the experimentally observed liquid length. It is plausible that, for the heaviest fraction, the mixing-limited assumption breaks down here; as discussed above, this would for physical reasons result in an underprediction by a mixing-limited model.

Moreover, comparing absolute values with this level of accuracy might not be useful in view of the uncertainty in experimental values, introduced by the choice of an intensity threshold in the determination of liquid lengths.

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It is slightly hard to judge from Figs. 2, 3 and 4 which model has the better overall predictive capability. To zoom in on the differences, Figs. 5, 6 and 7 show the deviation of modeled liquid lengths, obtained with the original and revised models, with respect to experimental data. This is done for three ambient density levels; to improve clarity and readability of the figures, the intermediate densities of 7.3 kg/m$^3$ and 30 kg/m$^3$ are left out.

Figure 5 shows the deviation between models and data for n-hexadecane. At the lowest density, differences between the original and revised models are negligible. However, there exists a clear temperature trend in the data: the error increases at lower temperatures, as was discussed above. For the highest density, this temperature trend in the deviation is reversed; for the intermediate density (15 kg/m$^3$, which is still low from a practical perspective) the temperature trend is clearly smaller.

Differences between the two model variants become significant for higher ambient densities. The revised model appears to have a better predictive capability at these density levels. Overall, both models show a significant spread in the errors. Since the overall error level can be “tuned” to some extent by revising the model constant $b$, it remains hard to conclude if either one of the models would be superior, based on this comparison. Still, since the revised model is physically more correct, it is to be preferred over the original model.
SUMMARY AND CONCLUSIONS

Siebers' mixing-limited scaling law for the so-called “liquid length” of a vaporizing diesel spray was critically evaluated, paying special attention to real gas effects. It was argued that the implementation of real gas effects in the original model, using separate compressibility factors for air and fuel, is not fully justified. Reconsidering first principle thermodynamics, a revised model was derived, in which real gas effects are incorporated in a more stringent way.

Furthermore, we have addressed the effect of real gas enthalpy (i.e. the impact of total pressure on enthalpy) on the mixing-limited liquid length scaling law. Implementation of departure functions based on the Peng-Robinson equation of state, however, has revealed that the effect of pressure on enthalpy can be neglected.

Comparing the results of the original and revised models with experimental data from Sandia National Laboratories it was found that, especially at the higher ambient density levels, liquid lengths computed with the revised model are significantly closer to the experimental data, for all three fuels considered (n-hexadecane, n-heptadecane and heptamethylnonane). Hence, correctly accounting for the (enhancing) effect of total pressure on saturated vapor pressure leads to a better predictive capability of Siebers' scaling law.

Figures 6 and 7 show the deviation in liquid length model predictions for HMN and n-heptadecane, respectively. Both figures basically show the same trends as Fig. 5. With a few exceptions, it can be seen that the revised model correlates the data better over the full temperature range. This certainly holds for the highest density, where real gas effects are most important: the original model is off by 18 to 40% in this range, whereas the revised model gives predictions ranging from −11 to +18% of experimental data. Predictive capability at low temperature and density remains poor, but can obviously not be expected to improve with inclusion of real gas effects. Overall, the observed trends for the three different fuels in Figs. 5, 6 and 7 are very consistent.
At the lowest ambient densities, the predictive capability of both the original and the revised model remains poor. Although at these conditions the main assumption of mixing-limited evaporation breaks down, this seems not to explain the observed overprediction of liquid lengths. If local inter-phase transport phenomena become limiting, this constitutes an extra barrier to evaporation, which would lead to an increase in liquid length. More research is required therefore to understand this model deficiency at these (low temperature and density) conditions. Yet, for conditions encountered in modern diesel engines, the high density range is more relevant.

REFERENCES


DEFINITIONS/ABBREVIATIONS

Roman symbols

\( a \) scaling constant for spray angle

\( b \) scaling constant for liquid length

\( B \) fuel-to-air mass flow rate ratio

\( C_a \) area contraction coefficient

\( d_0 \) nominal diameter of nozzle orifice

\( h \) enthalpy

\( L \) liquid length

\( m \) mass (with dot: mass flow rate)

\( M \) molar mass

\( p \) pressure

\( T \) temperature

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DEFINITIONS/ABBREVIATIONS
X
  mole fraction

Y
  mass fraction

Z
  compressibility factor

Subscripts
0
  pertaining to nozzle diameter

a
  air; (surface area in $C_a$)

f
  fuel

s
  saturation condition

Greek symbols

α
  idealized spray angle

ê
  real (measured) spray angle

ρ
  density

Abbreviations

EGR
  exhaust gas recirculation

HMN
  heptamethylnonane

SoI
  start of injection

TDC
  top dead center