

# Abstract

lends of gasoline, diesel fuel and ethanol ("dieseline") have shown promise in engine studies examining low temperature combustion using compression ignition. They offer the possibility of high efficiency combined with low emissions of oxides of nitrogen and soot. However, unlike gasoline or diesel fuel alone, such mixtures can be flammable in the headspace above the liquid in a vehicle fuel tank at common ambient temperatures. Quantifying their flammability characteristics is important if these fuels are to see commercial service. The parameter of most interest is the Upper Flammable Limit (UFL) temperature, below which the headspace vapour is flammable. In earlier work a mathematical model to predict the flammability of dieseline blends, including those containing ethanol, was developed and validated experimentally. It was then used to study the flammability of a wide variety of dieseline blends parametrically. Gasolines used in the simulations had DVPEs (Dry Vapor Pressure Equivalent) varying from 45 to 110 kPa. The parametric study revealed that the UFL temperatures of all alcohol-free dieseline blends were well correlated by blend DVPE, and the same correlation was found regardless of which gasoline or diesel fuels were used in the blends. For dieselines containing ethanol, the UFL temperatures could also be correlated using blend DVPE, but the UFL temperatures with ethanol present were different than for the alcohol-free blends at any given DVPE and varied with ethanol content. The results were presented graphically, from which UFL temperature could be estimated for any specific dieseline of interest. However, using the graphical data for broader analyses would be extremely time consuming. In the work reported here, explicit correlation equations have been derived that allow UFL temperature to be determined directly for dieseline blends with or without ethanol. The results have been shown to agree with the predictions of the full mathematical model on which they are based with an RMS error of less than 1°C. The equations can be used to quickly compare the UFL temperatures of a wide variety of dieseline formulations and to evaluate the impact of practical issues arising in-service, such as blending errors or regional variations.

# Introduction

ow Temperature Combustion (LTC) is a compression ignition approach that has the potential to avoid high engine-out oxides of nitrogen (NOx). Comparable particulate emissions to those associated with conventional diesel vehicles and emissions approaching Euro 6 levels have been demonstrated without the use of exhaust after-treatment. While such engines can run on conventional diesel fuels, there are advantages in using a fuel of lower cetane number where the longer ignition delay allows more time for mixing and optionally a higher compression ratio can be used for optimal efficiency. A more volatile fuel also assists in the fuel-air mixing process. [1, 2, 3, 4]

Market acceptance for LTC engines would be more likely if fuels currently available at the filling station could be used. However, in spite of recent progress, compression ignition (CI) operation on gasoline alone remains a formidable challenge. While good ignition can be achieved at medium and

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high loads, it is very difficult to achieve at the lower temperatures and pressures associated with idle and light load conditions without additional measures [<u>1</u>, <u>2</u>, <u>3</u>, <u>4</u>, <u>5</u>, <u>6</u>, <u>7</u>, <u>8</u>].

One possible solution would be to use both diesel and gasoline together, either in separate tanks or blended as a single fuel, termed "dieseline". Although this fuel is not currently available in filling stations, it could be supplied by blending at the fuel pump, which would be a less costly option than producing a completely separate fuel grade. This would provide a fuel with a lower cetane number and higher volatility than diesel, while avoiding the extreme ignitability problems of pure gasoline.

However, there is a concern with dieseline fuels due to their impact on the flammability of the air and fuel vapour mixture found in the headspace of a vehicle fuel tank. Diesel fuel has a relatively high boiling range and, under normal operating temperatures, the amount of fuel vapour in the tank is too low to support combustion. Gasoline is much more volatile than diesel so, at most ambient temperatures, the headspace vapours in the tank are too rich to burn. Depending upon the proportions of diesel and gasoline present in a dieseline mixture, the headspace vapour may be flammable over a range of ambient temperatures. Some dieseline blends of interest for LTC, particularly those with a low gasoline content, could produce a flammable headspace at the low ambient temperatures occurring in many markets.

The work presented here forms part of a larger study examining the flammability of potential dieseline blends in automotive fuel tanks [7, 8, 9]. Previously, a mathematical model for the flammability of blends of diesel fuel, gasoline and ethanol was validated experimentally [8]. The model was then used in a parametric study to assess fuel tank headspace flammability for a broad range of blends [9]. That work provided graphical data that can be used to determine the tank headspace flammability of dieseline blends formulated using gasolines having values of DVPE [10] from 45 kPa to 110 kPa and ethanol content from 0 to 50% by volume in the blend.

Although the graphical data presented in [9] can be used to determine the flammability of a particular case of interest, extracting data from the graphs is inconvenient for evaluating a large number of blends or examining the impact of systematic changes in formulation on the resulting flammability. However, the parametric study also showed that the flammability of dieseline blends, both with and without ethanol, can be correlated to blend DVPE. The purpose of the work presented here was to derive a set of explicit equations that would be simple to use and allow changes in headspace flammability to be quickly assessed quantitatively as dieseline formulation is varied over any desired range. It is hoped that this work will also help to raise awareness of the importance of flammability characteristics, when considering possible new fuels.

# Background

## **Flammability Limits**

For any given fuel there must be some minimum concentration of its vapour in air in order for the mixture to be flammable. Below that limiting value, referred to as the Lower Flammability Limit (LFL), the fuel/air mixture is too lean to support combustion. Similarly, there is some upper limit of concentration, referred to as the Upper Flammable Limit (UFL), above which the fuel/air mixture is too rich to burn.

The upper and lower flammability limits broaden slowly as temperature increases; however, over the range of ambient temperatures of interest for automobile fuel tanks, the two limits are essentially constant for any particular fuel vapour composition. Values of the LFL and UFL quoted in the literature for different compounds are typically those measured at room temperature.

# Flammability within a Fuel Tank

In a fuel tank the so-called "headspace" above the liquid level contains a quantity of air and fuel vapour such as shown in Figure 1.

The concentration of fuel vapour in the headspace at equilibrium depends only upon the temperature for any specific fuel. As temperature rises, the vapour pressure of the fuel increases, thereby increasing the amount of vapour in the headspace. <u>Figure 2</u> shows the situation generically.

As tank temperature increases from very cold conditions, vapour pressure increases, so fuel vapour concentration in the headspace increases. Eventually the concentration reaches









the lean limit, at which point the mixture in the headspace becomes flammable. The temperature at which this occurs at equilibrium is the Lower Flammable Limit (LFL) temperature. This is similar to the flash point temperature, but the apparatus, test procedures and pass/fail criteria are different for flash point and flammability limit tests. As a result, the flash points measured for liquid fuels are usually close to, but not necessarily exactly the same as, their LFL temperatures.

Above the LFL temperature the headspace contains a flammable mixture. However, if the tank temperature continues to rise, the concentration eventually reaches the Upper Flammable Limit (UFL) temperature and the mixture in the headspace then becomes too rich to burn.

For example, in the case of pure ethanol, the LFL temperature occurs at approximately  $-18^{\circ}$ C and the UFL temperature is reached at about  $+43^{\circ}$ C [<u>11</u>]. Therefore, the headspace in an ethanol fuel tank would be flammable at ambient temperatures from about  $-18^{\circ}$  to  $+43^{\circ}$ C.

## Flammability of Multi-Component Fuels

At equilibrium the flammability of a multi-component fuel vapour and air in a tank headspace is likewise determined by the tank temperature and the volatility of the liquid fuel. However, the composition of the fuel vapour, and hence its flammability, is determined by the partial pressures of all the volatile fuel components found in the vapour phase.

For most gasolines, even the UFL temperature occurs only at quite cold ambient conditions, although low volatility gasolines or those containing alcohol can have rich limits within the lower range of normal vehicle operating temperatures in cold climates.

In the case of diesel fuel, its low volatility results in tank headspace vapours that are normally too lean to burn; i.e. the LFL temperature is well above typical vehicle operating temperatures.

Combining diesel fuel and gasoline mixes a high volatility fuel with one of low volatility, thereby producing tank headspace vapours that potentially lie somewhere between the two extremes of too rich or too lean and hence could sustain combustion over a range of ambient temperatures. If ethanol is also a component, the non-ideal mixtures its forms with hydrocarbons complicates the prediction of the mixture flammability.

In practice, adding even small quantities of gasoline to diesel fuel can result in a flammable headspace mixture. Enough gasoline to give worthwhile advantages for LTC engines will likely result in LFL temperatures that occur only at extremely cold temperatures. LFL temperatures are therefore of little practical interest for such blends, so the requirement for modelling the flammability of dieseline mixtures is primarily to predict their UFL temperatures.

As was the case in the earlier results reported in [ $\underline{8}$ ,  $\underline{9}$ ], all the work presented here considers the fuel vapour and air mixture above the liquid in a fuel tank to be at equilibrium at a total tank pressure equal to the standard atmospheric pressure of 101.35 kPa. Modest deviations in total pressure do not affect the overall results significantly, especially the trends resulting from changing blend properties in a systematic way. Transient cases could be different and would need to be evaluated differently, although the equilibrium results would often be the starting point for the analysis.

To be most useful the flammability assessment for dieseline blends should require only readily available field data for the gasoline, diesel and ethanol components.

## Theory

## **Dieselines without Ethanol**

Because automotive fuel blends are usually specified in volumetric terms, calculating the DVPE of the dieseline blend requires the density and molecular weight of each component. These are needed to convert the volume percent of each component in the blend into the mole fractions necessary to calculate the blend vapour pressure at any temperature, including that of the DVPE (37.78°C). Field data will include the density, but not usually the molecular weight. Procedures to deal with such missing information will be provided in a later section.

Mole fractions for the ethanol-free gasoline and diesel components of the overall blend can be calculated as follows:

$$N_g = \rho_g Vol\%_g / M_g \tag{1}$$

$$N_d = \rho_d Vol\%_d / M_d \tag{2}$$

where

 $N_g$ = number of moles of gasoline in a unit volume of the blend

 $N_d$ = number of moles of diesel in a unit volume of the blend

 $\rho_{g}$  = density of the gasoline at 15°C

 $\rho_d$  = density of the diesel at 15°C

 $Vol\%_g$  = volume percent gasoline in the blend

 $Vol\%_d$  = volume percent diesel in the blend

 $M_{o}$ = Average Molecular Weight of the gasoline

 $\dot{M_d}$  = Average Molecular Weight of the diesel

1

The mole fractions of each are therefore:

$$X_g = N_g / \left( N_g + N_d \right) \tag{3}$$

$$X_d = N_d / \left( N_g + N_d \right) \tag{4}$$

where

 $X_g$  = mole fraction of gasoline in the blend  $X_d$  = mole fraction of diesel in the blend

As was shown in [8], the vapour pressure of gasoline can be simulated with reasonable accuracy by assuming that it consists of a limited number of significant volatile components with all remaining components treated as inert. These latter serve only to dilute the concentration of the volatiles in the fuel. When diesel fuel is added to gasoline, the diesel components are also treated as having negligible volatility. They add no significant additional volatiles but increase the concentration of inert components and thereby reduce the vapour pressure of the volatiles by reducing their mole fractions in the liquid phase at equilibrium. For this purpose the hydrocarbon-only mixture can be treated as an ideal mixture, so the vapour pressure at any temperature can be written as:

$$P_{volatiles} = X_{volatiles} P_{satv} \tag{5}$$

Where

 $P_{volatiles}$  = partial pressure of the volatiles at equilibrium  $X_{volatiles}$  = mole fraction of the volatiles in the liquid phase at equilibrium

 $P_{satv}$  = saturation pressure of the volatiles alone at the tank temperature

The DVPE test provides the vapour pressure corresponding to a vapour/liquid volume ratio of 4. At equilibrium, only a small portion of the volatiles is found in the vapour phase, with the bulk still in the liquid phase. For an exact determination of vapour pressure, an iterative solution is usually required to determine  $X_{volatiles}$  precisely for the liquid phase. However for the purpose of determining flammability, the small difference between the equilibrium concentration of volatiles in the liquid under DVPE conditions and their original concentration in the fuel as blended is very small and is within the uncertainty of the method overall. Consequently, by using the overall blend mole fractions, the DVPE of the dieseline can be shown to be:

$$DVPE_{HC \ blend} = DVPE_{gasoline} / \left(1 + \frac{\rho_d Vol\%_d / M_d}{\rho_g Vol\%_g / M_g}\right)$$
(6)

The field data that are readily available usually include the gasoline DVPE, the densities of the diesel and gasoline, and their volume percentages in the blend. However, the molecular weights are not usually available. For this purpose, it is suggested that  $M_d$  and  $M_g$  be taken as 190 and 90 respectively. This then allows the DVPE of the specified blend to be determined as a baseline case. If the additional uncertainty of the result due to these assumed values is of interest, then varying the two over their anticipated ranges will allow the differences in predicted DVPE and, ultimately, of UFL temperatures to be determined using the procedures described below.

# **Dieselines Containing Ethanol**

The mathematical model for these blends is described fully in  $[\underline{8}, \underline{9}]$ . Only the equations needed in order to use the correlations under various practical scenarios will be presented here.

Hydrocarbon/alcohol blends form non-ideal mixtures. Therefore, rather than an equation such as (5) the partial pressure of a component in the blend can be written:

$$P_i = \gamma_i X_i P_{isat} \tag{7}$$

where

 $P_i$  = vapour pressure of component *i* in the fuel mixture at equilibrium

 $\gamma_i$  = activity coefficient of component *i* in the blend

 $X_i$  = mole fraction of component *i* in the liquid phase of the blend at equilibrium

 $P_{i \, sat}$  = equilibrium saturation pressure of component *i* alone

The use of an activity coefficient in this equation is a simple method of accounting for non-ideality effects. Only two activity coefficients are required – one applicable to all the hydrocarbons and the other for ethanol.

In this method, the activity coefficient for each of the two components is a function only of the amount of the other component present in the binary mixture. They can be written as follows:

$$\gamma_{hydrocarbons} = e^{\frac{AX_{ethanol}^2}{T}}$$
(8)

$$\gamma_{ethanol} = e^{\frac{AX^2_{hydrcarbons}}{T}}$$
(9)

where

 $\gamma_{hydrocarbons}$  = single activity coefficient for all hydrocarbons in the blend

 $\gamma_{ethanol}$  = activity coefficient of the ethanol

 $X_{ethanol}$  =mole fraction of ethanol in the liquid at equilibrium

 $X_{hydrocarbons}$  = total mole fraction of hydrocarbon components in the liquid at equilibrium

$$= (1 - X_{ethanol})$$

T = absolute temperature (K). In this paper activity coefficients, when required, need to be calculated only for the DVPE conditions i.e. 310.93K (37.78°C).

A = the Margules coefficient

The Margules coefficient is a constant for any specific mixture of the two components, but varies for different concentrations of each. The following expression can be used to determine the value of the Margules coefficient A for these dieseline blends [8]:

$$A = 600 + 5.25[X_{ethanol}/(1 - X_{ethanol})]$$
(10)

Activity coefficients depend upon the liquid phase composition; therefore, they are not constant for a given overall fuel blend. They depend upon the composition of the liquid phase remaining when portions of each volatile component are found in the vapor phase. Activity coefficients are different for each particular temperature and the other factors that together determine the equilibrium conditions in the fuel tank. The key factor needed is how much ethanol is present in the liquid at equilibrium for any case of interest.

Using HC and EtOH as subscripts representing the hydrocarbons and ethanol respectively, the blend DVPE is the sum of the partial pressures of the two components.

$$DVPE_{blend} = P_{HC} + P_{EtOH} \tag{11}$$

The saturation pressure of each component at the DVPE temperature is its own DVPE. Using this and inserting (7) for each component into (11) then rearranging gives:

$$DVPE_{HC} = (DVPE_{blend} - \gamma_{EtOH}X_{EtOH}DVPE_{EtOH}) / \gamma_{HC}X_{HC} (12)$$

The mass of each component in the vapour phase under DVPE conditions is negligibly small. The values of the mole fractions in <u>equation (12)</u> are therefore approximately those in the original mixture.

# Results

# Conclusions from the Previous Parametric Study

When diesel fuel and gasoline are mixed together, the DVPE of the resulting blend depends upon the DVPE of the gasoline used and how much of each of the two components is in the blend. Figure 3 shows a typical example. In the case shown, the gasoline added to the diesel has a DVPE of 75 kPa.

An important conclusion drawn from the earlier study [9] was that the predicted UFL temperatures of all alcohol-free dieseline blends were well correlated by blend DVPE, and the same correlation was found regardless of which base gasoline was used in the blend. Similarly, the diesel properties had no effect upon the correlation for UFL temperature when plotted as a function of the DVPE of the resulting blends. Figure 4 shows those results.

The densities, molecular weights, volatility and proportions of gasoline and diesel fuel in the blend all affect the resulting blend DVPE. However, for any given DVPE, the UFL temperature of an alcohol-free blend is essentially the same regardless of what combinations of component properties

**FIGURE 3** Vapour Pressure of a Blend of Diesel Fuel and 75 kPA Gasoline







produced it. This reflects the empirical observation that the mixtures of light hydrocarbons usually found in the tank headspace for typical gasolines have an average rich limit of about 7–8% by volume. The modelling used detailed vapour pressure and flammability data for the components in the blends studied but the results summarized in Figure 4 show that those details are not needed to determine headspace flammability provided that the blend DVPE is known.

When ethanol is a component of dieseline blends, the flammability can again be correlated with blend DVPE. However. the correlation is different for such non-ideal blends than for dieseline composed only of hydrocarbons.

<u>Figure 5</u> compares the correlations found in [9] for a dieseline containing 10% ethanol with that for ethanol-free blends having the same DVPE.

Similar results are found for dieseline containing other amounts of ethanol but the resulting UFL temperatures are not the same for different amounts of ethanol in the blend.

The data in <u>Figure 5</u> can be presented in a more useful way: <u>Figure 6</u> shows the same data as <u>Figure 5</u>, but with an additional curve. The black curve again shows the UFL









temperatures for dieseline blends containing no ethanol, plotted against the DVPE of the blend. The solid red line again shows those results for dieseline blends containing 10% ethanol by volume, and again plotted against the DVPE of the blend. However, the dashed red line shows the same UFL temperature data for the 10% ethanol blend but plotted this time against the DVPE that the hydrocarbon components alone would have in each case if there were no ethanol present in the dieseline.

Although still different than the pure hydrocarbon correlation, the curve plotted using hydrocarbon DVPE is much closer to the curve for blends without ethanol. Each point on the dashed red line corresponds to a dieseline containing 10% ethanol that has the same DVPE as an ethanol-free hydrocarbon blend on the black curve. One way of interpreting the results shown in the figure is to consider that low DVPE ethanol blends (less than about 22 kPa in this case) have a lower UFL temperature than a hydrocarbon having the same DVPE. Above that point, 10% ethanol in a dieseline blend results in a higher UFL temperature compared to a hydrocarbon blend of the same DVPE. <u>Figures 7</u> to <u>10</u> show similar plots for dieseline blends containing other amounts of ethanol.







# FIGURE 9 Flammability of Dieseline Containing 30% Ethanol







The primary aim of this present work was to derive explicit equations that would allow disseline UFL temperatures to be calculated easily without iterative procedures. The data plotted against the DVPE of the hydrocarbon components in the blends alone provide a convenient basis for those equations. The process and the main observations from Figures 6-10 are as follows:

- The UFL for blends containing ethanol are considered as equivalent to the UFL for the hydrocarbon portion of the blend in its own right, plus a deviation to account for the presence of ethanol.
- The curves for blend UFL plotted against the DVPE of the hydrocarbon component alone are closer to the UFL values of the hydrocarbon but the variations differ depending upon how much ethanol is in the blend.
- the presence of ethanol can result in UFL temperatures that are either higher or lower than those of the hydrocarbon components alone.

• The differences depend upon both DVPE as well as the amount of ethanol in the blend. This reflects the two opposing tendencies involved. Ethanol tends to raise the vapour pressure but it has a higher UFL temperature than the hydrocarbons. The former effect tends to lower the UFL temperature of the blend whereas the latter tends to raise it. Which effect prevails depends upon the amount of ethanol in the blend.

## Equations for Estimating the Upper Flammability Limit Temperature

The basis for deriving correlating equations was first to determine a suitable correlating equation for the hydrocarbon-only data. Since vapour pressure is the underlying process, a correlation in the form of the Antoine Equation was considered. However, it was found that there was insufficient adjustability in that form to give satisfactory precision. Consequently, a less elegant but more accurate polynomial form was used, which gave acceptable precision in matching the correlation to the results of the model.

The data derived in [9] for dieseline blends formulated with different gasolines were then used to find the difference between the dieseline UFL temperature and that of its hydrocarbon components alone for each data point. Then equations were derived to account for the adjustments needed to the UFL temperature of the hydrocarbon-only portion of the dieseline due to both the amount of ethanol in the blends and the DVPE of the hydrocarbon-only portion.

The resulting general correlating equation is as follows:

$$T_{UFL} = f_1 (DVPE_{HC}) + f_2 (\% EtOH) \cdot f_3 (DVPE_{HC})$$
(13)

Where

 $T_{UFL}$  = Upper Flammable Limit Temperature for the blend [°C]

 $f_1(DVPE_{HC})$  is the correlating function for the curve of hydrocarbon-only blends that appears in each of the previous figures.

 $f_2(\%EtOH)$  is the correction factor to account for the volume percent ethanol in the blend

 $f_3(DVPE_{HC})$  is a factor to adjust  $f_2$  to account for the effect of  $DVPE_{HC}$ 

Each of the functions in Equation (13) is expressed as a polynomial of up to  $6^{\text{th}}$  order, for which the coefficients are given in <u>Table A1</u> of the <u>Appendix</u>. The general form for all three functions is as follows:

$$f = C_0 + C_1 \cdot arg + C_2 \cdot arg^2 + C_3 \cdot arg^3 + C_4 \cdot arg^4 + C_5 \cdot arg^5 + C_6 \cdot arg^6$$
(14)

Where *arg* is the argument of the respective function in <u>Equation (13)</u> - either  $DVPE_{HC}$  [kPa] or [volume]%*EtOH* in the blend

<u>Figure 11</u> compares the UFL temperatures determined by the correlation equations, compared to the predictions of the full mathematical model [9] for the blend.

The RMS value of the deviations between the two predictions of UFL temperature is approximately 0.9°C. The accuracy of the model predictions themselves is addressed below.





## Procedures for Estimating UFL Temperature

The procedures suggested in the following sections for determining the UFL temperatures of a dieseline blend are based on using the DVPE of the hydrocarbon component of the blend to find its own UFL temperature, then applying a correction factor for the deviation from that value if there is ethanol present in the blend. If the hydrocarbon DVPE is unknown, the requirement becomes to determine it. The processes described below allow the UFL temperature of a dieseline blend to be estimated for several situations in which different field data are available. The overall concept is the same - determine the hydrocarbon DVPE, then use the correlation in <u>Equation (13)</u> to find the UFL temperature.

In most cases, the volumetric percentages of gasoline, diesel fuel and ethanol in the proposed blend are specified and the usual field data are known for the gasoline and diesel components. Ethanol is assumed to have a density of 793.8 kg/m<sup>3</sup> and a molecular weight of 46. If there is already some ethanol in the gasoline then the volume percent ethanol in that gasoline component must be known and the quantity of ethanol in the dieseline blend used in <u>Equation (13)</u> must include the ethanol in the original gasoline as well as any that is added in formulating the dieseline.

The following examples illustrate the detailed procedures for using the correlation equations under various scenarios. A summary of these methods is shown in <u>Table A2</u> of the <u>Appendix</u>.

#### **Dieseline Blends without Ethanol**

**Case #1: Determine UFL Temperature given Dieseline Blend DVPE** For this simplest, alcohol-free case, the UFL temperature could be read directly from the graph in <u>Figure 4</u> but can now be calculated using <u>Equation (13)</u>. Only blend DVPE is needed - no data for either the gasoline or the diesel fuel being used in the blend are required. **Example 1:** A certain ethanol-free dieseline blend has a measured DVPE of 44.6 kPa. Since this blend contains no ethanol,  $f_2$  is zero and the UFL temperature becomes simply equal to  $f_1$ . Inserting the hydrocarbon DVPE gives an estimate for the UFL temperature of this blend of -7.77°C. The prediction given by the full mathematical model for this case is -8.00°C.

**Case #2: Determine UFL Temperature for an Ethanolfree Dieseline Blend given the Gasoline & Diesel Field Data** Given the DVPE of the gasoline, and densities of diesel and gasoline, the DVPE of the baseline blend can be calculated with <u>Equation (6)</u> using the values of diesel and gasoline molecular weights recommended above; namely, 190 and 90 respectively. The values of the molecular weights can then be varied over any expected range so as to assess the impact of such variations on the DVPE and hence on the UFL temperature. Similarly, volume percentages can be varied so as to examine the impact on the flammability of a dieseline blend due to errors or uncertainties in the proportions of the components used when producing the blend.

**Example 2:** A dieseline blend is formulated using 40% by volume of ethanol-free gasoline having a DVPE of 90 kPa and a density of 724.4 kg m<sup>-3</sup> and 60% diesel fuel having a density of 840 kg m<sup>-3</sup>.

Inserting these values plus the nominal assumed molecular weights of 90 and 190 respectively, <u>Equation (6)</u> predicts a DVPE for this all-hydrocarbon blend of 49.34 kPa. Inserting the value of DVPE <sub>HC</sub> into <u>Equation (13)</u> then gives a predicted UFL temperature for this blend of  $-10.5^{\circ}$ C. Using the full model with the properties of the 90 kPa surrogate gasoline described in [8] gives a predicted UFL temperature of  $-10.6^{\circ}$ C.

#### **Dieseline Blends Containing Ethanol**

**Case #3: Determine UFL Temperature given the proportions of diesel, ethanol and commercial gasoline in the blend** There are two possible scenarios in this case, depending upon whether the commercial gasoline used in the blend already contains some ethanol or not. Examples of each will be given.

**Example #3:** Determine UFL Temperature of a dieseline composed of 70% diesel (density 840 kg m<sup>-3</sup>), 10% ethanol and 20% ethanol-free gasoline. The gasoline has a DVPE of 60 kPa and a density of 745 kg m<sup>-3</sup>.

Equation (6) is used to determine DVPE of the hydrocarbon components alone. This requires the volume percentages of the ethanol-free gasoline and diesel. Note that the volume percentages in equation (6) must be those of the hydrocarbon portion of the mixture only - not those of the overall blend with ethanol. In this case the volume percentages of diesel and ethanol-free gasoline in the hydrocarbon phase in its own right are 77.8% and 22.2% respectively. Molecular weights are unknown so the suggested values of molecular weights of 190 and 90 for diesel and gasoline can be used in Equation (6). This then gives an estimated DVPE for the hydrocarbon components of 20.9 kPa. Inserting this into Equation (13) gives an estimated UFL temperature of 12.6°C. The full model for a similar case using surrogate gasoline G60[6], which has a slightly different molecular weight than the generic one assumed above, predicts a UFL temperature of 11.6°C.

**Example #4a:** Determine UFL Temperature of a dieseline composed of 60% diesel (density 840 kg m<sup>-3</sup>), 20% ethanol and 20% gasoline containing ethanol. The E10 gasoline has a DVPE of 60 kPa, a density of 760 kg m<sup>-3</sup> and an ethanol content of 10% by volume.

The first step is to find the DVPE of the hydrocarbon component of the gasoline.

The density of the gasoline ( $\rho_{gasoline}$ ) is known, as is the volume percent ethanol it contains. The subscript *ghc* below refers to the ethanol-free hydrocarbon component of the gasoline. The density of the hydrocarbon component can be found using:

$$\rho_{etOH} Vol_{etOH} + \rho_{ehc} Vol_{ehc} = 100 \rho_{easoline}$$
(15)

In this case, the volume percentage of hydrocarbon in the gasoline is 90% and that of the ethanol is 10%. Equation (15) gives the density of the hydrocarbon component itself as 757 kg m<sup>-3</sup>.

Equations (8) to (12) can now be used to obtain the DVPE of the hydrocarbon component of the gasoline but first the mole fractions of each of the components in the gasoline must be determined. Using Equations (1) to (4) for hydrocarbon and ethanol instead of gasoline and diesel, the mole fractions of the hydrocarbon component and ethanol in the gasoline are found to be 0.815 and 0.185 respectively.

Equations (8) to (12) then give the DVPE of the hydrocarbon component of the gasoline if no ethanol were present as 56.7 kPa.

The DVPE of the total hydrocarbon components of the dieseline can now be found. The volume percentage of gasoline hydrocarbon in the dieseline is 18% and diesel fuel is 60%. Their volume percentages in the hydrocarbon phase only are therefore 23.08% and 76.92% respectively. Using these values in <u>Equation (6)</u> along with the assumed molecular weights of 90 and 190 gives the DVPE of the hydrocarbon component of the dieseline blend as 20.6 kPa.

Using the hydrocarbon DVPE of 20.6 kPa and the total ethanol percentage of 22% in Equation (13) gives the estimated UFL temperature for this dieseline blend as 13°C. No direct comparison with the full model is readily available in this case because the correct mixture of volatiles and inert components would have to be determined for a gasoline such that it also had exactly the same density, molecular weight and DVPE as occurring in this example. However, a surrogate gasoline having the correct density and DVPE was formulated, but with a molecular weight of 79. The full model predicts a UFL temperature of 11.4°C for the dieseline blend of this example when using this gasoline. Using a gasoline molecular weight of 79 instead of the assumed value of 90 used above, the correlation predicts a UFL temperature of 12.8°C. The error using the correlation for this exact gasoline is therefore +0.2°C. Using the standard assumed gasoline molecular weight of 90 gave an error of +1.6°C. This difference illustrates the sensitivity of the predictions to molecular weight, which will be discussed further below.

Example 4a concerns a blend such as might be produced at a refinery. However, if dieseline were to be splash blended at a service station, there would not normally be any further ethanol added beyond what was already in the gasoline. Example 4b considers the same E10 gasoline blended with diesel but without the addition of further ethanol.

**Example #4b:** Determine UFL Temperature of a dieseline composed of 80% diesel (density 840 kg m<sup>-3</sup>) and 20% of the same E10 gasoline as in Example 4a.

The portion of the calculation that finds the DVPE of the hydrocarbon component of the gasoline is the same as in Example 4a, giving a DVPE for the gasoline hydrocarbons of 56.7 kPa.

The DVPE of the total hydrocarbon components of the dieseline can now be found. The volume percentage of gasoline hydrocarbon in the dieseline hydrocarbon is 18.37%, and diesel fuel is 81.63%. Using these values in Equation (6) along with the assumed molecular weights of 90 and 190 gives the DVPE of this splash blended dieseline as 17.0 kPa. Using this DVPE along with the 2% ethanol in Equation (13) gives a UFL temperature for this dieseline of 17.4°C.

**Case #4: Determine UFL Temperature for a Dieseline Blend given only the blend DVPE and Density.** This is the same situation as Case 1 except that there is ethanol in the blend in this case. To use the correlation <u>equation (13)</u> the DVPE of the hydrocarbon components in the mixture must be determined.

However, there is a difficulty here in that the molecular weight and density of the hydrocarbon phase are unknown. The hydrocarbon will consist of an unknown mixture of gasoline and diesel. For the same blend DVPE it could contain a relatively small amount of a high volatility gasoline or a larger amount of one that is less volatile. These differences result in different mole fractions in the liquid when ethanol is present and hence in different activity coefficients.

With an unknown hydrocarbon composition only an approximate UFL can be estimated. However, it was found that assuming an average molecular weight for the hydrocarbon of 143 and an average density of 795 kg m<sup>-3</sup> can give reasonable results in many cases, depending upon the DVPE of the gasoline. This is illustrated in the next example. This conclusion was drawn from a comparison between full model predications and this correlation method. The full model computed the UFL temperature for dieselines made up of the five surrogate gasolines in [9] with amounts of ethanol varying between 0 and 50%. The DVPE of the blends and their respective ethanol contents were then used to estimate the hydrocarbon DVPE, using the above assumed values of molecular weight and density, from which the UFL temperatures were then found.

Using this comparison, it was found that the simplified correlation using the assumed properties of the hydrocarbon phase is only slightly less precise than when using the known DVPE of the hydrocarbon phase. The RMS error was 0.97°C i.e. about 8% greater when DVPE of the hydrocarbon was estimated using these approximations compared to computations using the actual detailed components and their properties. In both cases, the variation in activity coefficients for dieselines having the same blend DVPE makes the scatter larger than for the pure hydrocarbon dieselines, for which the RMS error was 0.86°C. However, extreme values of DVPE may lead to greater discrepancies than this would suggest, as shown in Example 5 below.

**Example #5:** Determine the UFL Temperature of a dieseline containing 30% ethanol and having a DVPE of 40 kPa.

Using the suggested estimates for hydrocarbon density  $(795 \text{ kg m}^{-3})$  and molecular weight (143), the mole fractions of the hydrocarbon and ethanol are found to be 0.429 and 0.571 respectively. Equations (8) to (10) give activity coefficients of 1.89 for the hydrocarbon components and 1.43 for the ethanol. Equation (12) then gives a hydrocarbon DVPE of 33.25 kPa, from which Equation (13) gives a predicted UFL temperature of 1.3°C. Using gasolines having DVPE from 60-90 kPa the full model for dieseline blends predicts UFL temperatures of 0.6-1°C. However, the full model for this same DVPE but using gasoline having a DVPE of 45 kPa gives a UFL temperature of +2.2°C, whereas using a gasoline of DVPE 110 kPa gives -2.7°C. This shows that very low and very high DVPE gasolines in blends having the same resulting DVPE can have significantly different UFL temperatures. Using these blend hydrocarbon approximations to estimate UFK temperatures when the actual proportions of gasoline and diesel fuel are unknown has greater uncertainty if extreme values of DVPE may have been used to produce that known blend DVPE.

<u>Table A1</u> of the <u>Appendix</u> summarizes the procedures for using the correlation to predict UFL temperatures under the different scenarios illustrated in the examples above.

### Accuracy of Predictions and Sensitivity to Input Data

This section is included to highlight some issues that should be kept in mind when using the predictions for practical scenarios. A more detailed analysis of the accuracy of predicted UFL temperatures can be found in [8, 9].

The accuracy of a prediction depends on: 1) how well the model predicts the DVPE and; 2) how well the model then predicts the UFL temperature using that DVPE.

The model predicts the DVPE of blends of gasoline, diesel fuel and ethanol with an uncertainty up to 4% [8]. The resulting uncertainty in predicted UFL temperature would then be as much as 1.5°C at a DVPE of 90 kPa, and up to 2.5°C at a DVPE of 30 kPa.

However, the larger uncertainty in the predicted flammability for any specific case arises because the model uses literature values of upper temperature limits of flammability for the various pure compounds used in the simulations. This predicts trends well but the predicted UFL temperatures are very conservative; i.e. higher than would actually occur most practical cases. That is because the literature values reflect optimum combustion conditions, particularly upward flame propagation far from wall quenching effects. Under less than optimum combustion conditions (downward flame propagation or wall chilling) the actual UFL temperatures would be as much as 7–10°C colder than predicted by the model.

Regardless of the inherent uncertainty in the predicted UFL temperatures it was concluded that the model can be used to make a reasonable assessment of the trends resulting from changes in blend formulation and properties. In particular, comparisons can be made with gasolines and gasoline/ethanol blends on the same conservative basis, since those cases are included in the model simulations. Simply setting the diesel volume percentage to zero allows the flammability of gasolines or gasohols of any given DVPE to be examined on the same conservative basis as any particular dieseline of interest. Such comparisons are likely to be much more useful than simply predicting a particular UFL temperature under optimum combustion conditions.

The correlation equations add such a small additional factor to the uncertainty of the results that it is essentially negligible - less than 1°C in most cases for both hydrocarbononly blends as well as those containing ethanol. It is therefore concluded that the correlation equations can be used to assess the trends as satisfactorily as the full iterative model when different input data are varied.

However the results then depend upon the accuracy of the input data used. Blending of dieseline formulations using local commercial gasoline and diesel fuel will result in blends whose component properties are not all known, or which are different from those used when the proportions of the components were chosen originally. The user can investigate this easily by using the correlation equations to vary the input properties and study the resulting impact on predicted UFL temperature. Some examples will be given to illustrate the impacts.

A dieseline blend is specified as 10 volume percent of gasoline having a DVPE of 60 kPa, 20% ethanol and 70% diesel. Using the correlation equations the UFL temperature is found to be 12.6°C.

- If the blend were prepared using a gasoline meeting the DVPE requirement of 60 kPa but having a density 6% lower than the 745 kg m<sup>-3</sup> of the design specification, the predicted UFL temperature would rise by approximately 1.2°C. Higher gasoline densities would result in a greater mass of gasoline in the blend and hence a lower UFL temperature.
- If the diesel fuel density were 7% higher than the baseline value of 840 kg m<sup>-3</sup> then the UFL temperature would increase by 1.4°C. For comparison the full model prediction of the increase is 1°C.
- The field data available for gasoline and diesel usually will not include the molecular weight of either. Different combinations of light hydrocarbons in the gasoline can result in the same DVPE but different molecular weights. A difference in a component molecular weight changes the mole fractions in the liquid phase at equilibrium, and hence the vapour pressure and UFL temperature. If a very high gasoline molecular weight of 120 were assumed here instead of the baseline value of 90, the UFL temperature would rise by 3.4°C. If the diesel molecular weight were 170 instead of the 190 of the baseline case, the UFL temperature would rise by 1.7°C.
- If DVPE were reduced by 10% to 54 kPa the predicted UFL temperature would rise by 2.1°C.

# Summary

1. Explicit correlation equations have been derived that allow UFL temperature to be estimated for dieseline

blends with or without ethanol. The equations have been shown to agree with the predictions of the full mathematical model on which they are based with an RMS error of less than 1°C for UFL temperatures between -30°C and +30°C.

- 2. Like the mathematical model, the predictions are quite conservative, in that they are based on flammability limits corresponding to optimum combustion conditions. As shown in previous work (8) real world cases could be expected to have UFL temperatures lower by at least 7–10°C in most cases.
- 3. The equations can be readily programmed using spreadsheets or procedural programs to facilitate their use for assessing the UFL temperatures of a wide variety of dieseline formulations and for evaluating practical issues arising in-service.
- 4. The correlations are possibly most useful in examining trends when dieseline blend specifications and component properties are varied, rather than making a specific determination of UFL temperature. This is because they reflect the trends well despite the conservative estimates of UFL temperatures that they give. In particular, when the amount of diesel in the blend is set to zero, this gives the case for the gasoline on the same conservative basis. That can be used to compare the flammability of a dieseline blend to various gasolines already in use.
- 5. The correlations have been used to consider the sensitivity of UFL temperatures to some possible variations in densities and molecular weights of the hydrocarbon components and in the DVPE of the base gasoline used in the formulation. The impact was shown to be largest at low values of the DVPE of the hydrocarbon components of the blend. An estimate of such effects can be made easily using the correlations when the specific property variations expected are well defined.
- 6. It is hoped that this work raises awareness of the importance of flammability characteristics, when considering possible new fuels.

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## **Definitions**/Abbreviations

A - the Margules coefficient (Eqn 10)

arg - argument for algebraic functions used in  $\underline{equations\ 13}$  and  $\underline{14}$ 

**blend** - Referring to the blend of hydrocarbons in gasoline and/or diesel fuel

**dieseline** - A mixture of diesel fuel, gasoline and possibly ethanol

**DVPE** - Dry Vapor Pressure Equivalent (kPa)

- EtOH Referring to ethanol
- f algebraic functions used in equations 13 and 14
- HC Referring to the hydrocarbon components
- LTC Low Temperature Combustion

LFL - Lower Flammability Limit

 $M_d$  - Average Molecular Weight of the diesel

 $M_{g}$  - Average Molecular Weight of the gasoline

 $N_d$  - number of moles of diesel in a unit volume of the blend

 $N_g$  - number of moles of gasoline in a unit volume of the blend

NOx - oxides of nitrogen

 $P_i$  - vapour pressure of component i in the fuel mixture at equilibrium

 $P_{isat}$  - equilibrium saturation pressure of component *i* alone

 $P_{volatiles}$  - partial pressure of the volatiles at equilibrium

 $P_{satv}$  - saturation pressure of the volatiles alone at the tank temperature

RMS - Root mean square of errors

T - absolute temperature (K)

UFL - Upper Flammability Limit

*Vol*%<sub>*d*</sub> - volume percent diesel in the blend

*Vol*%<sub>g</sub> - volume percent gasoline in the blend

 $X_d$  - mole fraction of diesel in the blend

 $X_{ethanol}$  - mole fraction of ethanol in the liquid at equilibrium

 $X_g$  - mole fraction of gasoline in the blend

 $X_i$  - mole fraction of component *i* in the liquid phase of the blend at equilibrium

 $X_{hydrcarbons}$  - total mole fraction of hydrocarbon components in the liquid phase at equilibrium

 $X_{volatiles}$  - mole fraction of the volatiles in the liquid phase at equilibrium

 $\gamma_{ethanol}$  - activity coefficient of the ethanol

 $\gamma_{hydrocarbons}$  - single activity coefficient for all hydrocarbons in the blend

- $\gamma_i$  activity coefficient of component *i* in the blend
- $\rho_d$  density of the diesel at 15°C
- $\rho_{g}$  density of the gasoline at 15°C

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EXPLICIT EQUATIONS TO ESTIMATE THE FLAMMABILITY OF BLENDS OF DIESEL FUEL, GASOLINE AND ETHANOL

# Appendix



#### TABLE A1 Coefficients in the Correlation Equation

	Co	<b>C</b> <sub>1</sub>	<b>C</b> <sub>2</sub>	C <sub>3</sub>	C <sub>4</sub>	C₅	<b>C</b> <sub>6</sub>
f <sub>1</sub>	8.95413E+01	-7.44858E+00	2.78985E-01	-6.07073E-03	7.33348E-05	-4.57018E-07	1.14437E-09
<b>f</b> <sub>2</sub> if %EtOH=0	0	0	0	0	0	0	0
<b>f</b> <sub>2</sub> if DVPE <sub>HC</sub> <=20 & 0<%EtOH<=10	0	-4.40806E+00	7.98908E-01	-7.00812E-02	2.39390E-03	0	0
<b>f</b> <sub>2</sub> if DVPE <sub>HC</sub> <=20 & %EtOH>10	-9.89867E+00	-5.14490E-02	1.79400E-03	0	0	0	0
<b>f</b> <sub>2</sub> if DVPE <sub>HC</sub> >20 & %EtOH>0	1.04207E-01	2.90263E-01	-1.31394E-02	2.27509E-04	-1.34341E-06	0	0
<b>f</b> <sub>3</sub> if DVPE <sub>HC</sub> <=20	2	-0.1	0	0	0	0	0
f3 if 20 <dvpehc<40< td=""><td>-1.67230E+00</td><td>9.36900E-02</td><td>-6.25320E-04</td><td>0</td><td>0</td><td>0</td><td>0</td></dvpehc<40<>	-1.67230E+00	9.36900E-02	-6.25320E-04	0	0	0	0
<b>f</b> <sub>3</sub> if DVPE <sub>HC</sub> >=40	1	0	0	0	0	0	0

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#### EXPLICIT EQUATIONS TO ESTIMATE THE FLAMMABILITY OF BLENDS OF DIESEL FUEL, GASOLINE AND ETHANOL

TABLE A2	Summary of	of Processes	for Estimating l	JFL Temperature
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Example	Known	Assumed Property Values	Process to find UFL temperature	Comments
1	DVPE <sub>blend</sub> , no ethanol content	none	$DVPE_{HC}$ =DVPE <sub>blend</sub> ; Eqn (13) with $f_2$ =0 gives UFL Temperature	
2	Vol% gasoline & diesel in blend; field data <sup>1</sup> for diesel and ethanol-free gasoline	Assume baseline values of MW <sub>gasoline</sub> =90 MW <sub>diesel</sub> =190	Eqn <u>(6)</u> gives DVPE <sub>HC</sub> Eqn <u>(13)</u> with f <sub>2</sub> =0 gives UFL Temperature	MW can be varied as required to assess impact on UFL compared to baseline case
3	Vol% gasoline, diesel & ethanol in blend; field data <sup>1</sup> for diesel and ethanol-free gasoline	Assume baseline values of MW <sub>gasoline</sub> =90 MW <sub>diesel</sub> =190	Eqn <u>(6)</u> gives DVPE <sub>HC</sub> Eqn <u>(13)</u> gives UFL Temperature	Use Vol% in HC portion only in Eqn (6); MW can be varied as required to assess impact on UFL compared to baseline case
4	Vol% gasoline, ethanol and diesel in blend; field data <sup>1</sup> for diesel and gasoline containing ethanol	Assume baseline values of $MW_{gasoline}$ =90 $MW_{diesel}$ =190 $MW_{EtOH}$ =46 $\rho_{EtOH}$ =793.8 kg/m <sup>3</sup> DVPE <sub>EtOH</sub> =15.95 kPa	Eqn (15) gives $\rho_{ghc}^2$ Eqns (1) to (4) with EtOH replacing diesel give mole fractions in gasoline; Eqns (8)-(10) & (12) give DVPE <sub>ghc</sub> Eqn (6) gives DVPE <sub>HC</sub> Eqn (13) gives UFL Temperature	Use Vol% in HC portion of dieseline in Eqn (6); Use total EtOH vol% in Eqn (13) MWs and densities can be varied as required to assess impact on UFL compared to baseline case
5	DVPE <sub>blend</sub> , ethanol Vol%	$\label{eq:rho_Hc} \begin{split} \rho_{Hc} = & 795 \text{kg/m}^3 \\ \rho_{EtOH} = & 793.8 \text{ kg/m}^3 \\ \text{MW}_{Hc} = & 143 \\ \text{MW}_{EtOH} = & 46 \\ \text{DVPE}_{EtOH} = & 15.95 \text{ kPa} \end{split}$	Eqns ( <u>1</u> ) to ( <u>4</u> ) with EtOH replacing diesel give mole fractions in blend; Eqns ( <u>8</u> )-( <u>10</u> ) & ( <u>12</u> ) give DVPE <sub>HC</sub> Eqn ( <u>13</u> ) gives UFL Temperature	$MW_{\text{HC}}$ and $\rho_{\text{HC}}$ can be varied as required to assess impact on UFL compared to baseline case

<sup>1</sup>field date available are assumed to be density, DVPE and ethanol volume % for gasoline and diesel density

<sup>2</sup> subscript ghc refers to the hydrocarbon component of the gasoline

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