Blended E85-diesel fuel droplet heating and evaporation

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# **ABSTRACT**

The multi-dimensional quasi-discrete (MDQD) model is applied to the analysis of heating and evaporation of mixtures of E85 (85% volume fraction of ethanol and 15% volume fraction of gasoline) with diesel fuel, commonly known as ‘E85-diesel’ blends, using the universal quasi-chemical functional group activity coefficients model for the calculation of vapor pressure. The contribution of 119 components of E85-diesel fuel blends is taken into account under conditions representative of diesel engines. Our results show that high fractions of E85-diesel fuel blends have a significant impact on predicted droplet lifetimes and surface temperatures. For instance, droplet lifetime and surface temperature for a blend of 50% volume fraction of E85 and 50% volume fraction of diesel are 23.2% and up to 3.4% less than those of pure diesel fuel, respectively. The application of the MDQD model has improved the computational efficiency significantly with minimal sacrifice to accuracy. This approach leads to a saving of up to 86.4% of CPU time compared to the approach taking into account the contributions of all 119 components.

**Keywords:** Activity coefficient, Diesel, Ethanol, Evaporation, Fuel blends, Gasoline, Heating.

# **INTRODUCTION**

Diesel engines are the main power source of passenger cars and heavy duty vehicles because of their relatively high efficiency.1 Due to the common greenhouse emissions (mainly carbon oxides and nitrogen oxides) associated with diesel engines, and depletion of fossil fuels, many investigations have been carried out on possible replacement of diesel fuel with alternatives such as ethanol.2–6 Ethanol and ethanol-gasoline mixtures have been shown to be suitable for blending with diesel fuels.1,7 It is known that mixtures with up to 15%[[2]](#footnote-2) ethanol and 85% diesel can be used in standard diesel engines without significant impact.8 Also, it has been reported in ref 9 that ethanol can be blended with diesel fuel at up to 20% ethanol.

The most common blends of diesel fuel are not pure ethanol but 85% ethanol and 15% gasoline (E85) fuels.1,7,10,11 The addition of 15% gasoline to ethanol is commonly used to improve the low temperature properties of the mixture and the cold start in diesel engines.10,12 The results of experimental research1 have shown that the presence of E85 in diesel fuel leads to a noticeable reduction in nitrogen oxides. This mixture, however, has also led to a noticeable increase in the ignition delay and increase in the production of carbon monoxides. The combustion temperature decreases with increasing E85/diesel fuel fraction, and the brake efficiency slightly increases for higher E85/diesel fuel fractions.10 These effects, however, need to be treated cautiously; for instance, the addition of 20% E85 can lead to up to 16% increase in nitrogen oxides.10

So far research on E85-diesel fuel blends has been focused on the physical properties, exhaust toxic emissions and ignition of this fuel.1,7,10,11 The impact of such blends, accounting for full fuel compositions, and their detailed species chemical structure and properties, on droplet heating and evaporation has not been investigated to the best of our knowledge. The importance of modelling multi-component fuel droplet heating and evaporation processes in automotive applications has been highlighted in many studies.13–16 In most of the previous studies (e.g., see refs 17–19) either the Infinite Thermal Conductivity/Infinite Diffusivity (ITC/ID) and the distillation curve models were used, or the diffusivity was ignored altogether and the single component model was used (see ref 17 for details). However, rapid evaporation of light components at the surface of the droplet leads to a high gradient of component mass fractions inside the droplet. Moreover, the temperature gradient near the droplet surface at the initial stage of droplet heating is expected to be very high due to the high ambient temperature. A number of models have been developed within the last decade to study these processes, including the Discrete Component (DC) model.13,20,21 The version of the DC model described in the latter references and used in our paper is based on the analytical solutions to the heat transfer and species diffusion equations. The DC model is generally applicable to cases when the number of components is relatively small. The application of this model, however, is expected to be computationally expensive when the number of components exceeds several dozen. To address this problem, the multi-dimensional quasi-discrete (MDQD) model has been suggested.22 In this model, a large number of components is replaced with a much smaller number of components/quasi-components (C/QC) without losing the main features of the DC model. This approach allows one to reduce the computational time by up to 96% without substantial loss of accuracy,23–25 which is important for the implementation of the model into commercial CFD codes (e.g., see26–28). As with the above-mentioned version of the DC model, the MDQD model is based on the analytical solutions to the heat transfer and species diffusion equations using the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) models. The latter models allow one to take into account the recirculation inside the droplets due to their relative movement, and its effect on the droplet average surface temperature and species mass fractions within a one-dimensional model.29,30 The DC and MDQD models have been applied to gasoline, diesel, biodiesel and their blends.22–24,30–35 This paper is focused on the analysis of blended E85-diesel fuel droplets. In contrast to most previous studies, where Raoult’s law was assumed to be valid (i.e. the activity coefficient (AC) was assumed to be unity), the authors of36 took into account the contributions of non-unity AC using the universal quasi-chemical functional group activity (UNIFAC) model. In this paper, the analysis of ref 36 is generalized to the case of blended E85-diesel droplets using the DC and MDQD models. The basic equations and the compositions of fuel, used in our analysis, are described in Section 2. The validation of the model and the results predicted, using the DC and MDQD models, are presented and discussed in Section 3. The main results are summarized in Section 4.

# **MODEL AND FUEL COMPOSITIONS**

Our analysis is based on the DC and MDQD models assuming that all processes are spherically symmetric. The effects of droplet relative motion are accounted for using the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) models.37 The basic equations used in our analysis and fuel compositions are summarized in the following sections.

## **DROPLET HEATING**

The process of heating of mono- and multi-component spherical droplets is described by the transient heat conduction equation for temperature in the liquid phase:38,39

, (1)

where is time, is the distance from the center of the droplet, *T* is the temperature, and is the effective thermal diffusivity,40–42

, (2)

is the specific heat capacity, is the density, and is the Effective Thermal Conductivity (ETC), defined by the following expression:40

, (3)

takes into account the effect of recirculation inside droplets as:42,43

, (4)

, is the Reynolds number, is the maximum surface velocity inside droplet, and is the friction drag coefficient, is the Prandtl number, is the gas velocity, is the droplet velocity, and are liquid dynamic viscosity and thermal conductivity, respectively, and is the Spalding mass transfer number defined later.13 The initial and boundary conditions for Eq. (1) are introduced as:

, (5)

where *T*s = *T*s(*t*) is the droplet surface temperature, is the droplet radius, *T*g = *T*g(*t*) is the ambient gas temperature, and *h*= *h*(*t*) is the convective heat transfer coefficient, linked with the Nusselt number Nu by the following expression:

, (6)

where is the gas thermal conductivity. To take into account the effect of evaporation, the gas temperature *T*g is replaced with the effective temperature *T*eff:44

, (7)

where *L* is the latent heat of evaporation and is the rate of change of droplet radius due to evaporation, which is taken from previous time step and is estimated using Equation (31). At any given time step, is assumed constant in the analytical solutions and is updated at the end of the time step , as: , where the value of is controlled by the droplet evaporation and swelling (see Equations (29)-(31)). Remembering the physical background of the problem, we are only interested in the solution which is twice continuously differentiable in the whole domain. This implies that should be bounded for .

Assuming constant , the analytical solution to Equation (1), applied for the time step gives the following expression for the temperature at the end of each time step, when :45

, (8)

where , , , ,, .

A set of positive eigenvalues, > 0 (the trivial solution is not considered), is found from the solution to the following equation:

. (9)

In the limit the prediction of Expression (8) reduces to the one which follows from the model based on the assumption that (Infinite Thermal Conductivity (ITC) model).46 The value of Nu for an isolated moving droplet is estimated using the following equation:40

, (10)

where, is the Spalding heat transfer number:

, (11)

where is the specific heat capacity at constant pressure of the fuel vapor,

, (12)

is the power spent on the droplet heating, are the evaporation rates of species , and *.* The effects of the interaction between droplets are ignored (simplified models for these effects are discussed in refs 41,47,48). The analysis of the evaporation process in this paper is based on the assumption that a mixture of vapor species and air can be treated as a separate gas (see Equation (22)).

## **SPECIES DIFFUSION IN THE LIQUID PHASE**

Assuming that the processes inside droplets are spherically-symmetric, equations for mass fractions of liquid species can be presented as:49

, (13)

where = 1,2,3,… refers to species, is the effective liquid species mass diffusivity (assumed to be the same for all species and estimated based on the average characteristics of the liquid fuel) linked with the liquid diffusivity via the following equation:

, (14)

where coefficient is approximated as:

, (15)

is the liquid Schmidt number, is the liquid kinematic viscosity, and is the same as described in Equation (2.4). As in the case of the ETC model, the liquid fuel transport properties and liquid velocity just below the surface of the droplet were used for calculating. The model based on Equations (13)-(15) is known as the Effective Diffusivity (ED) model.40,42

The analytical solution to Equation (13) was obtained, subject to the following boundary condition:37

, (16)

and the initial condition , where are liquid components’ mass fractions at the droplet’s surface,

, (17)

is the droplet evaporation rate, the calculation of which is discussed in Section 2.3 (see Equation (22)). As in the case of Equation (1), we are only interested in a solution which is continuously twice differentiable in the whole domain. This implies that should be bounded for . Moreover, the physical meaning of , as the mass fraction, implies that .

Assuming that species concentrations in the ambient gas are equal to zero (this assumption can be critical when applied to confined spaces), the values of can be found from the following relation:49–51

. (18)

The conditions and α = const. can always be guaranteed for sufficiently small time steps. The analytical solution to Equation (13) can be presented as:49

, (19)

where and are determined from the solutions to equations and , respectively, ,

, (20)

is obtained from Equation (8), replacing with , and:

, (21)

The model, based on Equation (13) is known as the Discrete Component (DC) model.

## **DROPLET EVAPORATION**

In the case of multi-component droplets the problem of modelling droplet evaporation is complicated by the fact that different species diffuse at different rates; and the evaporation rate of one of the species is affected by the evaporation rate of other species.47,49 Following refs 37,52, the relative diffusion of components in the gas phase is ignored and the analysis of evaporation of multi-component droplets will be based on the following expression for (as in the case on mono-component droplets):

, (22)

where is the binary diffusion coefficient of vapor in gas (air), = is the total density of the mixture of vapor and gas, is the density of the ambient gas, is the Spalding mass transfer number defined as:53

(23)

is the vapor mass fraction, and are densities of vapor in the vicinity of droplets surfaces and at a large distance from them, is the Sherwood number approximated for isolated droplets by the following expression:40

, (24)

is the droplet Reynolds number based on the droplet diameter, is the Schmidt number for the gas phase, is the same as in (10) but with replaced with .20 and are linked by the following equation:40

, (25)

, (26)

is the Lewis number, and

, (27)

, (28)

are modified Sherwood and Nusselt Numbers for non-evaporating droplets, respectively. The ratio is equal to 1 for stationary droplets. This ratio was sometimes assumed equal to 1 for slowly moving droplets.37,49 Such an assumption turned out to be too crude in some cases; hence, Expressions (27) and (28) were used to estimate based on Equation (26). Note that .

When calculating the value of , both droplets evaporation and thermal swelling during the time step were taken into account:54

, (29)

where is the change of droplet radius due to thermal expansion/contraction calculated based on the following equation:54

, (30)

and are average droplet temperatures at the beginning and the end of the time-step. The value of is controlled by droplet evaporation:37

, (31)

where is given by Equation (22).

## **SPECIES MASS FRACTIONS AT THE SURFACE OF DROPLET**

To calculate the species evaporation rate and the values of the evaporation rate of species based on Equation (18), the values of need to be calculated. The latter depend on the molar fraction of species in the vapor phase in the immediate vicinity of the droplet surface ():55

|  |  |
| --- | --- |
| , | (32) |

where is the molar fraction of the *i*th species in the liquid phase near the droplet surface, and is the saturated vapor pressure of the *i*th species. In the case when (i.e. for the *i*th species), is the total (ambient) pressure, is the activity coefficient (AC), and is the fugacity coefficient. It has been shown in some studies (e.g., see ref .56) that the non-ideality mainly originates from the liquid phase, while it is very low at the gas phase for the parameters used in this study. Hence the fugacity coefficient can be assumed equal to unity, which justifies the applicability of the ideal gas law used in our analysis. In the limit when, Equation (32) describes the Raoult’s law.57

In contrast to previous studies, we have calculated without approximation, using the multi-component universal quasi-chemical functional group activity coefficients (UNIFAC) model.36 We have used the latter model for the prediction of the activity coefficients of 119 components of E85-diesel fuel blends, which is estimated as:58,59

|  |  |
| --- | --- |
|  | (33) |

where , , is the area fraction of each molecule in the mixture, is the segment (volume) fraction of each molecule, is the volume parameter, is the surface parameter, , is the area fraction of group , is the molar fraction of group , and and are the Van der Waals volumes and surface areas for each group, respectively.[[3]](#footnote-3) is the residual AC of group *k* in the mixture and is the residual AC of group in a reference solution containing only molecules of type is the interaction and temperature dependent coefficient, is the group-interaction parameter between groups *m* and *n*, is the interface temperature. The implementation of the UNIFAC model for the vapor pressure predictions has been validated for a highly non-ideal mixture (ethanol/gasoline).36

All liquid properties are calculated for the average temperature inside droplets. All gas properties are calculated for the reference temperature, where and are droplet surface, and ambient gas temperatures respectively. The ambient air density is calculated using the ideal gas law. The enthalpy of evaporation and saturated vapor pressure are estimated at.

## **SOLUTION ALGORITHM**

These are the main steps of the numerical algorithm for the hydrodynamic model used in our analysis:

1. Assume an initial distribution of temperature and mass fractions of species inside the droplet or use the distributions obtained at the previous time step (in our case both initial distributions were assumed homogeneous). Recalculate the molar fractions of species into mass fractions of species.
2. Calculate the values of liquid thermal conductivity and effective thermal conductivity of the droplet.
3. Calculate species partial pressures and molar fractions in the gas phase, using Equation (32).
4. Calculate the value of the Spalding mass transfer number, using Equation (23).
5. Calculate the values of liquid heat capacity and diffusivity of the mixture of vapor species in the air, and species evaporation rates (), using Equation (18).
6. Calculate the value of the Spalding heat transfer number, using the iteration process based on Equations (25)-(28).
7. Calculate the values of the Nusselt and Sherwood numbers for isolated droplets, using Equations (10) and (24).
8. Calculate the values of and using Equations (27) and (28).
9. Calculate the rate of change of droplet radius, using Equations (29)-(31).
10. Calculate the effective temperature, using Equation (7).
11. Calculate the distribution of temperature inside the droplet based on Equation (8), using 44 terms in the series.
12. Calculate the distribution of species inside the droplet based on Equation (19), using 33 terms in the series. Note that the chosen number of terms adversely affects the accuracy of predicted distribution of species if this number is much less than 33. This effect is much weaker for the distribution of temperature in droplets.
13. Recalculate the droplet’s radius at the end of the time step. If this radius is negative then the time step is reduced and the calculations are repeated. If the ratio of this radius to the initial radius is less than an *à priori* chosen small number, , then the remaining part of the droplet is assumed to be evaporated with all liquid species transferred into the gas phase with a corresponding decrease in gas temperature. If this ratio is greater than then go to the next step.
14. Recalculate the distributions of temperature and species for the new droplet radius (e.g., , where are droplet radii at the beginning and the end of the time step, is the new used at the second time step, and are the values of temperature at the end of the first time step).
15. Return to Step 1 and repeat the calculations for the next time step.

## **FUEL COMPOSITIONS**

The same diesel fuel as in 19 and gasoline for advanced combustion engines (FACE C) were used in our analysis. Diesel fuel consists of 98 hydrocarbon components, including the following mole fractions of components: 40.0556% alkanes, 14.8795% cycloalkanes, 7.6154% bicycloalkanes, 16.1719% alkylbenzenes, 9.1537% indanes & tetralines, 8.6773% naphthalenes, 1.5647% tricycloalkanes (represented by a characteristic component C19H34), 1.2240% diaromatics (represented by a characteristic component C13H12), and 0.6577% phenanthrenes (represented by a characteristic component C14H10). The composition of gasoline fuel (simplified from 83 to 20 hydrocarbons based on the similarity in chemical structure and thermodynamic and transport properties of components)20 includes the following mole fractions of the components: 28.61% n-alkanes, 65.19% iso-alkanes, 4.25% alkylbenzene, 0.10% indanes (represented by C9H10), 1.49% cycloalkanes (represented by C8H16), and 0.35% olefins (represented by C9H18). Water free bio-ethanol (anhydrous) is used to represent ‘ethanol’ in the fuel mixtures. Ethanol is assumed to be completely miscible in diesel (this assumption is open to question, especially for high mass fractions of ethanol due to the differences in chemical structures and characteristics of ethanol and diesel fuel).60,61

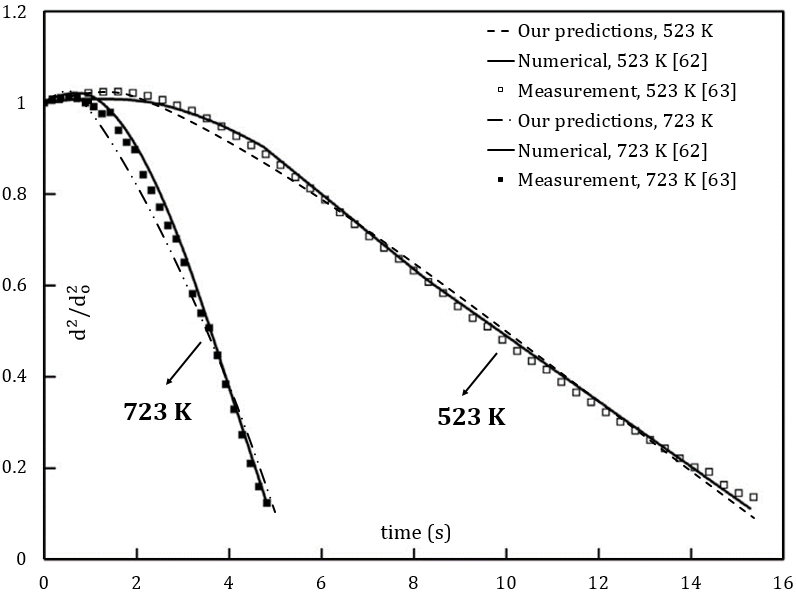
The following volume fractions of E85 (85% ethanol and 15% gasoline)/diesel fuels are considered: 0% E85 (i.e. pure diesel), E85-5, E85-20, E85-50, E85-80, and E85 (E85-X refers to a mixture of X% volume fraction of E85 fuel and (100-X)% volume fraction of diesel fuel). The thermodynamic and transport properties of gasoline, diesel and ethanol are inferred from refs 19,20,27.

# **RESULTS**

# **MODEL VALIDATION**

The results of the application of the DC model to investigate the evaporation of diesel fuel were validated against experimental data and verified with numerical simulations.62,63 In these papers, diesel fuel was approximated by the following components (based on their mass fractions): 8% toluene (C7H8), 11% decane (C10H22), 21% dodecane (C12H26), 27% tetradecane (C14H30), 17% hexadecane (C16H34), and 16% octadecane (C18H38). Droplets with initial diameters 0.86 mm (for ambient gas temperature K), and 0.84 mm (for ambient gas temperature K) and initial temperature of 300 K were suspended at the tip of a quartz fiber.62,63 The droplet relative velocities in a chamber with ambient pressure of 1 atm were 0.3 m/s. The ETC/ED model was used.62 Note that the authors of the latter paper state that ‘the droplet temperature and composition were assumed to be uniform’, which would contradict their claim that they use the ETC/ED model. We believe that this is a typo in their paper and they refer to droplet surface temperature and composition.

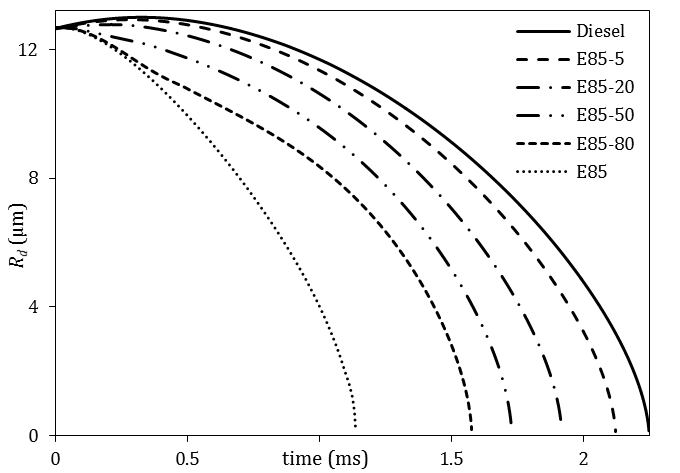
The time evolutions of the normalized squared droplet diameters, predicted using our model, were compared with the numerical results presented in ref 62 and experimental data provided in ref 63. The results of the comparison are shown in Figure 1. As follows from this figure, the predictions of our code are reasonably close to the numerical and experimental data.



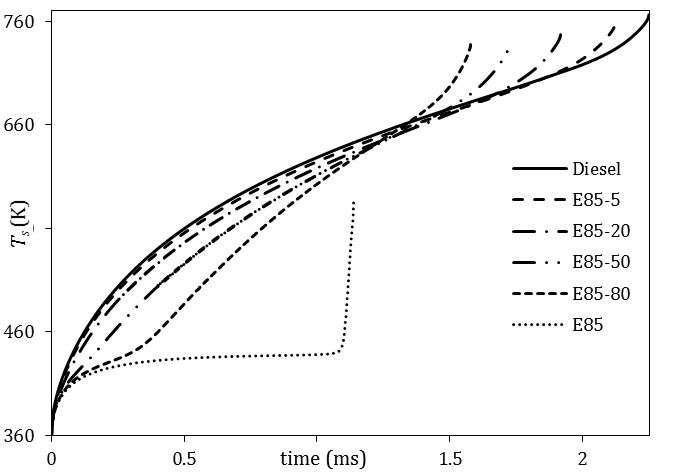
**Figure 1.** Predicted and experimentally measured normalized squared diameters of diesel fuel (represented by 6 components)62,63 droplets.

# **PREDICTIONS OF THE DC MODEL**

The impacts of various volume fractions of E85-diesel fuel blends on droplet heating and evaporation were investigated using the DC model, where the contribution of 98, 119 and 21 components were considered for pure diesel, E85-diesel blends and pure E85, respectively. The partial vapor pressures of the components of the blended fuel were calculated taking into account the non-unity ACs for up to 119 components using the UNIFAC model. As in refs 32,64, the initial droplet radius was taken equal to and its constant axial velocity in still air and initial temperature were assumed equal to m/s and K, respectively. The ambient air pressure and temperature were assumed constant and equal to bar and K, respectively. The evolution of droplet radii and surface temperatures versus time for various E85/diesel fuel blends are shown in Figures 2 and 3, respectively.



**Figure 2.** Droplet radii versus time for various E85-diesel blends. The droplet with the initial radius 12.66 µm and initial homogeneous temperature 360 K was assumed to be moving with constant velocity of 10 m/s in still air. Ambient pressure and temperature were taken equal to 30 bar and 800 K, respectively.



**Figure 3.** Droplet surface temperature versus time for various E85-diesel blendsfor the same ambient conditions and input parameters as in Figure 2.

As follows from Figure 2, droplet lifetime for pure diesel is longer than that for any blend. It decreases as the E85 fraction increases. The difference in droplet lifetime for E85-5 compared to pure diesel is 5.7%. This difference reaches 49.5% for pure E85. This significant reduction in droplet lifetime is ascribed to the fact that E85 is more volatile than pure diesel and has a saturation vapor pressure of 207 kPa (at), while it is only 2.3 kPa for pure diesel at the same temperature.

The droplet surface temperatures versus time for various E85-diesel blends are shown in Figure 3. As can be seen from this figure, droplet surface temperature decreases with increasing E85 volume fractions. For E85-5, it is up to 0.78% less than that of pure diesel. This reduction is increased to 3.4% for E85-50 and reached 23.4% for pure E85. This difference is attributed to the fact that the heat capacity of ethanol is noticeably higher than that of diesel fuel. In agreement with the previous studies,30,65,66 droplet surface temperature does not show plateau profiles due to the diffusion of multi-component composition of droplets.

The temperature distribution inside the droplet is shown in Figure 4 at time instants 0.02, 0.3, 0.5 and 1 ms. As can be seen from this figure, the temperature difference between the droplet center and its surface can reach up to 9.2 %. Note that the results shown in Figure 4 should be treated with care for the case of non-zero droplet relative velocities since the ETC/ED models were primarily developed for correct prediction of the surface temperature and species mass fractions in this case.

**Figure 4.** Temperature inside droplet () versus normalized distance from the center of droplet for E85-5 blend at time instants 0.02, 0.3, 0.5 and 1 ms.

The distillation characteristics of E85-5 and pure E85, estimated using the ETC/ED models, with the same ambient conditions as in Figures 2-4, are presented in Figure 5. As can be seen from this figure, the percentage volume recovered as distillate, for pure E85, starts at and ends (100% recovered) at which is less than the average boiling point of pure E85 at. For the E85-5 mixture, the percentage volume recovered starts at and ends at. The sudden increase in droplet surface temperature without any volume recovered, for the latter mixture, is ascribed to the fact that the lighter components (E85) are evaporated and the remaining are only the diesel components which start evaporating at. This behavior is similar to that described in ref 17.

**Figure 5.** Droplet surface temperature versus percentage volume recovered as distillate for E85-5 and pure E85 using the ETC/ED models.

To assess the impact of the non-ideality of the liquid phase on the estimated droplet lifetimes and surface temperatures, a comparison between the results based on the two activity coefficients (the unity and UNIFAC) for E85-5 and E85-20 fuel blends is shown in Figure 6. One can see from this figure that the droplet lifetime predicted using the UNIFAC model is about 3.6% shorter than that based on the assumption of a unity activity coefficient. This is attributed to the fact that the non-ideal mixture entails a higher vapor pressure, due to the presence of ethanol, compared to the ideal mixture. Hence, the faster evaporation rates and shorter droplet lifetimes.

**Figure 6.** Droplet surface temperatures and radii versus time for E85-5 and E85-20 blendsfor the same ambient conditions and input parameters as in Figures 2-5.

The time evolution of selected 9 (out of 119) species mass fractions for E85-5 blend is shown in Figure 7. The selected components are: C10H22, C19H40, C27H56 (the alkane group), C20H40, C27H54 (the cycloalkane group), C12H18, C24H42 (the alkylbenzene group), C8H18 (iso-octane in gasoline) and C2H5OH (ethanol). As can be seen from this figure, the mass fractions of the lighter components in the blend (e.g., C2H5OH, C8H18 and C10H22) decrease monotonically with time, while the mass fractions of the intermediate components initially increase at the expense of lighter components and then decrease with time. The mass fractions of heavy components (C27H56 and C27H54) increase until they become the dominant ones, although they have very small fractions initially.

**Figure 7.** The plots of surface mass fractions of 9 representative components of the E85-5 blend versus time. The plots for the following components are shown: C1012H22 (1), C19H40 (2), C27H56 (3), C20H40 (4), C27H54 (5), C12H18 (6), C24H42 (7), C8H18 (8) and C2H5OH (9). The same ambient conditions and input parameters as in Figures 2-6 were used.

# **PREDICTIONS OF THE MDQD MODEL**

The MDQD model was applied to the analysis of E85-5 droplets. The input parameters and ambient conditions were the same as those used for the analysis based on the DC model. The impacts of various approximations of 119 components of E85-5 blends on the predictions of droplet radii and surface temperatures are shown in Figures 8 and 9, respectively. These approximations are: 90, 63, 45, 20 and 16 components/quasi-components (C/QC) (see Appendix B for details). As can be seen from these figures, the errors in droplet lifetimes and surface temperatures predicted by the model using 90 C/QC are 0.38% and up to 0.26%, respectively, less than those predicted using the DC model taking into account the contributions of all components. These errors increase to 0.99% and up to 0.39% for droplet lifetimes and surface temperatures, respectively, when the blend is approximated by 63 C/QC. They further increased to 7.16% for droplet lifetime and up to 2.90% for the droplet surface temperature, when 16 C/QC were used. These errors are rather large for many engineering applications. At the same time, it was found that the approximation of the blend by 20 C/QC under-predicts the droplet lifetimes and surface temperatures by up to 3.58% and up to 2.90%, respectively, which is acceptable in most engineering applications.

**Figure 8.** Droplet radii versus time for six approximations of E85-5: 119 components using the DC model, and 90, 63, 45, 20 and 16 C/QC (numbers near the curves) using the MDQD model, for the same ambient conditions and input parameters as in Figures 2-7.

**Figure 9.** Droplet surface temperature versus time for six approximations of the E85-5 blend: 119 components using the DC model, and 90, 63, 45, 20, and 16 C/QC (numbers near the curves) using the MDQD model, for the same ambient conditions and input parameters as in Figures 2-8.

The computational efficiency of the MDQD model in terms of the required CPU time is illustrated in Table 1. For example, the approximation of 119 E85-5 components by 20 components/quasi components can reduce CPU time by up to 82.7%. A workstation with Intel(R) Core(TM) i5-3337U, 1.80 GHz, 2 Core(s) and 8 GB RAM was used. The time step was set as 1 µs.

**Table 1.** The impact of reducing the number of components on CPU time.

|  |  |  |
| --- | --- | --- |
| number of C/QC | CPU time (sec) | Diff % |
| 119 | 1816 | - |
| 90 | 1360 | 25.1 |
| 63 | 955 | 47.4 |
| 45 | 687 | 62.2 |
| 20 | 314 | 82.7 |
| 16 | 247 | 86.4 |

# **CONCLUSION**

The heating and evaporation of blended E85-diesel fuel droplets are investigated in conditions representative of diesel engines. It is shown that E85-diesel blended fuel droplets have shorter lifetimes than those of pure diesel. Higher fractions of E85 result in up to 49.5% shorter droplet lifetimes and up to 23.4% lower droplet surface temperatures than those of pure diesel.

The activity coefficient for prediction of the species mass fraction at the surface of the droplet is calculated using the UNIFAC model. In the case of the E85-5 blend, the assumption of an ideal-mixture with a unity activity coefficient (i.e. Raoult’s law is valid) is shown to lead to over-prediction of droplet lifetimes by up to 3.6%, compared to the case when the UNIFAC activity coefficient is used.

It is shown that replacing 119 components of the blended fuel with 20 components/quasi-components reduces CPU time by up to 83% with less than 3.6% and 2.9% under-predicted droplet lifetimes and surface temperatures, respectively, compared to the prediction of the model taking into account the contribution of all 119 components.

# **APPENDIX A. THE APPROXIMATION OF FIVE STRUCTURE GROUPS OF THE ACs**

The values of parameters and for five of the groups in the composition of diesel fuel (bicycloalkanes, naphthalenes, tricycloalkanes, diaromatics and phenanthrenes) are not provided anywhere to the best of our knowledge. We have approximated the structure of these groups of molecules to the nearest available structures for which the values of parameters and are known, taking into account the number of groups in each molecule. For example, when the aromatic molecule C10H14 (its structure group is available in literature) has 1 aromatic ring (C6), 3 CH2 and 1 CH3 (the numbers 1, 3 and 1 refer to which is the number of groups in molecule), the diaromatic molecule C12H16 is approximated by 2 aromatic rings (C6). In other words, the diaromatic group is approximated by 2 single aromatic groups, as shown in Table 2. This approximation allowed us to predict the activity coefficients for all components of the E85-diesel fuel blend.

**Table 2.** The approximation of the missing structure groups for the predictions of the ACs.

|  |  |  |
| --- | --- | --- |
| Group name | Group structure | |
| Missing group | Approximation |
| Bicycloalkanes |  | (CH2)3CH3 |
| The bicyclo-C10H18 is approximated by Cyclo-C6, 3 CH2 and 1 CH3. | |
| Naphthalenes |  | CH2CH=CHCH3 |
| The naphthalenes C10H8 is approximated by 1 aromatic C6, 1 CH2, 1 CH=CH and 1 CH3. | |
| Tricycloalkanes |  | CH3 |
| The tricycloalkane C14H24 is approximated by 2 cyclo C6 and 2 CH3. | |
| Diaromatics | CH3  CH3 |  |
| The diaromatic C12H16 is approximated by 2 aromatic C6. | |
| Phenanthrenes |  | CH3 |
| The phenanthrene C14H11 is approximated by 2 aromatic C6 and 2 CH3 | |

Note that both and are functions of bond distances, bond angles, contact distances, and shapes that are characteristic of the structure group.67 Thus, the interaction between the five groups is expected to be different. These structure groups (filled circles) have not previously been presented in the literature, to the best of our knowledge, and we have approximated them to the nearest available groups.

# **APPENDIX B. APPROXIMATIONS OF THE E85-DIESEL FUEL BLEND**

**Table 3.** The numbers of components/quasi-components (C/QC) (top line), and the compositions of C/QCs (carbon numbers), used in the MDQD model for approximating E85-5.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Group** | | **119** | **90** | **63** | **45** | **20** | **16** |
| Alkanes (Diesel) | | 8 | 8 | 8 | 8.91 (C8–C9) | 10.33 (C8–C12) | 10.33 (C8–C12) |
| 9 | 9 | 9 |
| 10 | 10 | 10 | 10.38 (C10–C11) |
| 11 | 11 | 11 |
| 12 | 12 | 12 | 12.49 (C12–C13) |
| 13 | 13 | 13 | 15.05 (C13–C17) | 15.05 (C13–C17) |
| 14 | 14 | 14 | 14.54 (C14–C15) |
| 15 | 15 | 15 |
| 16 | 16 | 16 | 16.52 (C16–C17) |
| 17 | 17 | 17 |
| 18 | 18 | 18 | 18.52 (C18–C19) | 19.38 (C18–C22) | 19.38 (C18–C22) |
| 19 | 19 | 19 |
| 20 | 20 | 20 | 20.39 (C20–C21) |
| 21 | 21 | 21 |
| 22 | 22 | 22 | 22.33 (C22–C23) |
| 23 | 23 | 23 | 23.84 (C23–C27) | 23.84 (C23–C27) |
| 24 | 24 | 24 | 24.34 (C24–C25) |
| 25 | 25 | 25 |
| 26 | 26.42 (C26-C27) | 26.42 (C26-C27) | 26.42 (C26-C27) |
| 27 |
| Cycloalkanes (Diesel) | | 10 | 10 | 10.74 (C10-C11) | 10.74 (C10-C11) | 12.56 (C10–C15) | 12.56(C10–C15) |
| 11 | 11 |
| 12 | 12 | 12.43 (C12-C13) | 12.43 (C12-C13) |
| 13 | 13 |
| 14 | 14 | 14.47 (C14-C15) | 14.47 (C14-C15) |
| 15 | 15 |
| 16 | 16 | 16.49 (C16-C17) | 16.49 (C16-C17) | 18.29 (C16–C21) | 18.29 (C16–C21) |
| 17 | 17 |
| 18 | 18 | 18.51 (C18-C19) | 18.51 (C18-C19) |
| 19 | 19 |
| 20 | 20 | 20.35 (C20-C21) | 20.35 (C20-C21) |
| 21 | 21 |
| 22 | 22 | 22.26 (C22-C23) | 22.26 (C22-C23) | 22.98 (C22–C27) | 22.98 (C22–C27) |
| 23 | 23 |
| 24 | 24 | 24.37 (C24-C25) | 24.37 (C24-C25) |
| 25 | 25 |
| 26 | 26.42 (C26-C27) | 26.42 (C26-C27) | 26.42 (C26-C27) |
| 27 |
| Bicycloalkanes (Diesel) | | 10 | 10.60 (C10-C11) | 10.60 (C10-C11) | 11.1 (C10–C12) | 14.74(C10–C25) | 14.74(C10–C25) |
| 11 |
| 12 | 12.40 (C12-C13) | 12.40 (C12-C13) |
| 13 | 13.86 (C13–C15) |
| 14 | 14.43 (C14-C15) | 14.43 (C14-C15) |
| 15 |
| 16 | 16.57 (C16-C17) | 16.57 (C16-C17) | 17.09 (C16–C18) |
| 17 |
| 18 | 18.60 (C18-C19) | 18.60 (C18-C19) |
| 19 | 19.31 (C19–C21) |
| 20 | 20.32 (C20-C21) | 20.32 (C20-C21) |
| 21 |
| 22 | 22.41 (C22-C23) | 22.41 (C22-C23) | 22.92 (C22–C25) |
| 23 |
| 24 | 24.42 (C24-C25) | 24.42 (C24-C25) |
| 25 |
| Alkylbenzenes (Diesel) | | 8 | 8 | 8.86 (C8-C9) | 8.86 (C8–C9) | 10.207 (C8–C13) | 10.72(C8–C16) |
| 9 | 9 |
| 10 | 10 | 10.15 (C10-C11) | 10.15 (C10–C11) |
| 11 | 11 |
| 12 | 12 | 12.26 (C12-C13) | 12.26 (C12–C13) |
| 13 | 13 |
| 14 | 14 | 14.42 (C14-C15) | 14.42 (C14–C15) | 16.23 (C14–C19) |
| 15 | 15 |
| 16 | 16 | 16.45 (C16-C17) | 16.47 (C16–C17) |
| 17 | 17 | 19.02 (C17–C24) |
| 18 | 18 | 18.38 (C18-C19) | 18.38 (C18-C19) |
| 19 | 19 |
| 20 | 20 | 20.41 (C20-C21) | 20.41 (C20-C21) | 21.08 (C20–C24) |
| 21 | 21 |
| 22 | 22 | 22.74 (C22-C24) | 22.74 (C22-C24) |
| 23 | 23.49(C23-C24) |
| 24 |
| Indanes & tetralines (Diesel) | | 10 | 10 | 10.51 (C10-C11) | 11.41 (C10–C13) | 12.49 (C10–16) | 13.83 (C10–C22) |
| 11 | 11 |
| 12 | 12 | 12.47 (C12-C13) |
| 13 | 13 |
| 14 | 14 | 14.45 (C14-C15) | 15.34 (C14–C17) |
| 15 | 15 |
| 16 | 16 | 16.46 (C16-C17) |
| 17 | 17 | 18.61 (C17–C22) |
| 18 | 18 | 18.39 (C18-C19) | 19.24 (C18–C22) |
| 19 | 19 |
| 20 | 20 | 20.57 (C20-C22) |
| 21 | 21.32 (C21-C22) |
| 22 |
| Naphthalenes (Diesel) | | 10 | 10 | 10.56 (C10-C11) | 11.53 (C10–C15) | 12.39 (C10–C20) | 12.39 (C10–C20) |
| 11 | 11 |
| 12 | 12 | 12.35 (C12-C13) |
| 13 | 13 |
| 14 | 14 | 14.44 (C14-C15) |
| 15 | 15 |
| 16 | 16 | 16.42 (C16-C17) | 17.90 (C16–C20) |
| 17 | 17 |
| 18 | 18 | 18.98 (C18-C20) |
| 19 | 19.51 (C19-C20) |
| 20 |
| Diesel | Tricycloalkane | 19 | 19 | 19 | 19 | - | - | |
| Diaromatic | 13 | 13 | 13 | 13 | - | - |
| Phenanthrene | 14 | 14 | 14 | 14 | - | - |
| N-alkanes (gasoline) | | 4 | 5.24 (C4-C12) | 5.24 (C4-C12) |  | 5.24 (C4-C12) | 5.24 (C4-C12) |
| 5 |  |
| 6 | 5.24 (C4-C12) |
| 10 |  |
| 12 |  |
| Iso-alkanes (gasoline) | | 4 | 7.37 (C4-C8) | 7.37 (C4-C8) |  | 7.37 (C4-C8) | 7.41 (C4-C11) |
| 5 |  |
| 6 | 7.37 (C4-C8) |
| 7 |  |
| 8 |  |
| 9 | 9.74 (C9-C11) | 9.74 (C9-C11) | 9.74 (C9-C11) | 9.74 (C9-C11) |
| 10 |
| 11 |
| Alkylbenzenes (gasoline) | | 8 | 9.07 (C8-C11) | 9.07 (C8-C11) | 9.07 (C8-C11) | 9.07 (C8-C11) | 9.07 (C8-C11) |
| 9 |
| 10 |
| 11 |
| Gasoline | Indane | 9 | - | - | - | - | - |
| Cycloalkane | 8 | - | - | - | - | - |
| Olefin | 9 | - | - | - | - | - |
| Ethanol | | 2 | 2 | 2 | 2 | 2 | 2 |

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# **REFERENCES**

(1) Sarjovaara, T.; Larmi, M. Dual Fuel Diesel Combustion with an E85 Ethanol/Gasoline Blend. *Fuel* **2015**, *139*, 704–714.

(2) EPA, U. US Environmental Protection Agency http://www.epa.gov/ (accessed Mar 29, 2018).

(3) US Department of Energy. Ethanol Blends https://www.eia.gov/energyexplained/index.php?page=biofuel\_ethanol\_use#tab2 (accessed Apr 20, 2018).

(4) Li, D.; Zhen, H.; Xingcai, L.; Wu-gao, Z.; Jian-guang, Y. Physico-Chemical Properties of Ethanol–Diesel Blend Fuel and Its Effect on Performance and Emissions of Diesel Engines. *Renew. Energy* **2005**, *30* (6), 967–976.

(5) Chin, J.-Y.; Batterman, S. A.; Northrop, W. F.; Bohac, S. V.; Assanis, D. N. Gaseous and Particulate Emissions from Diesel Engines at Idle and under Load: Comparison of Biodiesel Blend and Ultralow Sulfur Diesel Fuels. *Energy Fuels* **2012**, *26* (11), 6737–6748.

(6) Liu, X.; Wang, H.; Yao, M. Experimental and Modeling Investigations on Soot Formation of Ethanol, *n* -Butanol, 2,5-Dimethylfuran, and Biodiesel in Diesel Engines. *Energy Fuels* **2017**, *31* (11), 12108–12119.

(7) Tutak, W. Bioethanol E85 as a Fuel for Dual Fuel Diesel Engine. *Energy Convers. Manag.* **2014**, *86*, 39–48.

(8) Torres-Jimenez, E.; Jerman, M. S.; Gregorc, A.; Lisec, I.; Dorado, M. P.; Kegl, B. Physical and Chemical Properties of Ethanol–Diesel Fuel Blends. *Fuel* **2011**, *90* (2), 795–802.

(9) Padala, S.; Woo, C.; Kook, S.; Hawkes, E. R. Ethanol Utilisation in a Diesel Engine Using Dual-Fuelling Technology. *Fuel* **2013**, *109*, 597–607.

(10) Tutak, W.; Lukács, K.; Szwaja, S.; Bereczky, Á. Alcohol–Diesel Fuel Combustion in the Compression Ignition Engine. *Fuel* **2015**, *154*, 196–206.

(11) Curran, S.; Hanson, R.; Wagner, R. Effect of E85 on RCCI Performance and Emissions on a Multi-Cylinder Light-Duty Diesel Engine; 2012.

(12) Jeuland, N.; Montagne, X.; Gautrot, X. Potentiality of Ethanol As a Fuel for Dedicated Engine. *Oil Gas Sci. Technol.* **2004**, *59* (6), 559–570.

(13) Sazhin, S. S. *Droplets and Sprays*; Springer: London, 2014.

(14) Al Qubeissi, M. *Heating and Evaporation of Multi-Component Fuel Droplets*; WiSa: Stuttgart, 2015.

(15) Stojkovic, B. D.; Sick, V. Evolution and Impingement of an Automotive Fuel Spray Investigated with Simultaneous Mie/LIF Techniques: *Appl. Phys. B* **2001**, *73* (1), 75–83.

(16) Sirignano, W. A. Fuel Droplet Vaporization and Spray Combustion Theory. *Prog. Energy Combust. Sci.* **1983**, *9* (4), 291–322.

(17) Hallett, W. L. H.; Beauchamp-Kiss, S. Evaporation of Single Droplets of Ethanol–Fuel Oil Mixtures. *Fuel* **2010**, *89* (9), 2496–2504.

(18) Laurent, C.; Lavergne, G.; Villedieu, P. Continuous Thermodynamics for Droplet Vaporization: Comparison between Gamma-PDF Model and QMoM. *Comptes Rendus Mécanique* **2009**, *337* (6–7), 449–457.

(19) Burger, M.; Schmehl, R.; Prommersberger, K.; Schäfer, O.; Koch, R.; Wittig, S. Droplet Evaporation Modeling by the Distillation Curve Model: Accounting for Kerosene Fuel and Elevated Pressures. *Int. J. Heat Mass Transf.* **2003**, *46* (23), 4403–4412.

(20) Sazhin, S. S. Modelling of Fuel Droplet Heating and Evaporation: Recent Results and Unsolved Problems. *Fuel* **2017**, *196*, 69–101.

(21) Sazhin, S. S.; Al Qubeissi, M.; Xie, J.-F. Two Approaches to Modelling the Heating of Evaporating Droplets. *Int. Commun. Heat Mass Transf.* **2014**, *57*, 353–356.

(22) Sazhin, S. S.; Al Qubeissi, M.; Nasiri, R.; Gun’ko, V. M.; Elwardany, A. E.; Lemoine, F.; Grisch, F.; Heikal, M. R. A Multi-Dimensional Quasi-Discrete Model for the Analysis of Diesel Fuel Droplet Heating and Evaporation. *Fuel* **2014**, *129*, 238–266.

(23) Al Qubeissi, M.; Sazhin, S. S.; Turner, J.; Begg, S.; Crua, C.; Heikal, M. R. Modelling of Gasoline Fuel Droplets Heating and Evaporation. *Fuel* **2015**, *159*, 373–384.

(24) Al Qubeissi, M.; Sazhin, S. S.; Elwardany, A. E. Modelling of Blended Diesel and Biodiesel Fuel Droplet Heating and Evaporation. *Fuel* **2017**, *187*, 349–355.

(25) Al Qubeissi, M.; Sazhin, S. S.; Al-Esawi, N. Models for Automotive Fuel Droplets Heating and Evaporation. In *the Institute for liquid atomization and spray systems (ILASS)*; Universitat Politècnica València, Spain, 2017; pp 1044-1051.

(26) Rybdylova, O.; Al Qubeissi, M.; Braun, M.; Crua, C.; Manin, J.; Pickett, L. M.; Sercey, G. de; Sazhina, E. M.; Sazhin, S. S.; Heikal, M. A Model for Droplet Heating and Its Implementation into ANSYS Fluent. *Int. Commun. Heat Mass Transf.* **2016**.

(27) Rybdylova, O.; Poulton, L.; Al Qubeissi, M.; Elwardany, A. E.; Crua, C.; Khan, T.; Sazhin, S. S. A Model for Multi-Component Droplet Heating and Evaporation and Its Implementation into ANSYS Fluent. *Int. Commun. Heat Mass Transf.* **2018**, *90*, 29–33.

(28) Zaripov, T. S.; Rybdylova, O.; Sazhin, S. S. A Model for Heating and Evaporation of a Droplet Cloud and Its Implementation into ANSYS Fluent. *Int. Commun. Heat Mass Transf.* **2018**, *97*, 85–91.

(29) Al Qubeissi, M. Predictions of Droplet Heating and Evaporation: An Application to Biodiesel, Diesel, Gasoline and Blended Fuels. *Appl. Therm. Eng.* **2018**, 136, 260-267.

(30) Al Qubeissi, M.; Al-Esawi, N.; Sazhin, S. S.; Ghaleeh, M. Ethanol/Gasoline Droplet Heating and Evaporation: Effects of Fuel Blends and Ambient Conditions. *Energy Fuels* **2018**, *32* (6), 6498–6506.

(31) Al Qubeissi, M.; Sazhin, S. S.; Crua, C.; Turner, J.; Heikal, M. R. Modelling of Biodiesel Fuel Droplet Heating and Evaporation: Effects of Fuel Composition. *Fuel* **2015**, *154*, 308–318.

(32) Al Qubeissi, M.; Al-Esawi, N.; Sazhin, S. S. Droplets Heating and Evaporation: An Application to Diesel-Biodiesel Fuel Mixtures. In *the Institute for liquid atomization and spray systems (ILASS)*; Universitat Politècnica València, Spain, 2017; pp. 1060-1067.

(33) Al Qubeissi, M.; Al-Esawi, N.; Kolodnytska, R. Atomization of Bio-Fossil Fuel Blends. In *Advances in Biofuels and Bioenergy*; Nageswara-Rao, M., Soneji, J. R., Eds.; InTech, 2018.

(34) Al-Esawi, N.; Al Qubeissi, M.; Sazhin, S. S. The Impact of Fuel Blends and Ambient Conditions on the Heating and Evaporation of Diesel and Biodiesel Fuel Droplets. In *15th International Heat Transfer Conference (IHTC16)*; Begellhouse: Beijing, China, 2018; (in press).

(35) Al Qubeissi, M.; Sazhin, S. S. Blended Biodiesel/Diesel Fuel Droplet Heating and Evaporation. In *the Institute for liquid atomization and spray systems (ILASS)*; Brighton, UK, 2016; Vol. DHE-01, p 179.

(36) Al-Esawi, N.; Al Qubeissi, M.; Sazhin, S. S.; Whitaker, R. The Impacts of the Activity Coefficient on Heating and Evaporation of Ethanol/Gasoline Fuel Blends. *Int. Commun. Heat Mass Transf.* **2018**, *98*, 177–182.

(37) Sazhin, S. S. Advanced Models of Fuel Droplet Heating and Evaporation. *Prog. Energy Combust. Sci.* **2006**, *32* (2), 162–214.

(38) Carslaw, H. S. *Conduction of Heat in Solids*, 2nd ed.; Clarendon Press; Oxford University Press: Oxford: New York, 1986.

(39) Kartashov, E. M. *Analytical Methods in Heat Transfer Theory in Solids*; Vysshaya Shkola: Moscow, 2001.

(40) Abramzon, B.; Sirignano, W. A. Droplet Vaporization Model for Spray Combustion Calculations. *Int. J. Heat Mass Transf.* **1989**, *32* (9), 1605–1618.

(41) Elwardany, A. E. Modelling of Multi-Component Fuel Droplets Heating and Evaporation. PhD thesis, University of Brighton: UK, 2012.

(42) Abramzon, B.; Sazhin, S. S. Convective Vaporization of a Fuel Droplet with Thermal Radiation Absorption. *Fuel* **2006**, *85* (1), 32–46.

(43) Sirignano, W. A. *Fluid Dynamics and Transport of Droplets and Sprays*; Cambridge University Press: Cambridge, UK, 2010.

(44) Sazhin, S. S.; Kristyadi, T.; Abdelghaffar, W. A.; Heikal, M. R. Models for Fuel Droplet Heating and Evaporation: Comparative Analysis. *Fuel* **2006**, *85* (12–13), 1613–1630.

(45) Sazhin, S. S.; Krutitskii, P. A.; Abdelghaffar, W. A.; Sazhina, E. M.; Mikhalovsky, S. V.; Meikle, S. T.; Heikal, M. R. Transient Heating of Diesel Fuel Droplets. *Int. J. Heat Mass Transf.* **2004**, *47* (14–16), 3327–3340.

(46) Sazhin, S. S.; Krutitskii, P. A. A Conduction Model for Transient Heating of Fuel Droplets. In *proceedings of the 3rd ISAAC Congress*; World Scientific: River Edge, NJ, 2003; pp 1231–1240.

(47) Maqua, C.; Castanet, G.; Grisch, F.; Lemoine, F.; Kristyadi, T.; Sazhin, S. S. Monodisperse Droplet Heating and Evaporation: Experimental Study and Modelling. *Int. J. Heat Mass Transf.* **2008**, *51* (15–16), 3932–3945.

(48) Sazhin, S. S.; Elwardany, A. E.; Krutitskii, P. A.; Deprédurand, V.; Castanet, G.; Lemoine, F.; Sazhina, E. M.; Heikal, M. R. Multi-Component Droplet Heating and Evaporation: Numerical Simulation versus Experimental Data. *Int. J. Therm. Sci.* **2011**, *50* (7), 1164–1180.

(49) Sazhin, S. S.; Elwardany, A.; Krutitskii, P. A.; Castanet, G.; Lemoine, F.; Sazhina, E. M.; Heikal, M. R. A Simplified Model for Bi-Component Droplet Heating and Evaporation. *Int. J. Heat Mass Transf.* **2010**, *53* (21–22), 4495–4505.

(50) Continillo, G.; Sirignano, W. A. Unsteady, Spherically-Symmetric Flame Propagation Through Multicomponent Fuel Spray Clouds. In *Modern Research Topics in Aerospace Propulsion*; Angelino, G., Luca, L. D., Sirignano, W. A., Eds.; Springer New York, 1991; pp 173–198.

(51) Faeth, G. M. Evaporation and Combustion of Sprays. *Prog. Energy Combust. Sci.* **1983**, *9* (1–2), 1–76.

(52) Deprédurand, V.; Castanet, G.; Lemoine, F. Heat and Mass Transfer in Evaporating Droplets in Interaction: Influence of the Fuel. *Int. J. Heat Mass Transf.* **2010**, *53* (17–18), 3495–3502.

(53) Spalding, D. B. *Convective Mass Transfer: An Introduction*; Edward Arnold Publ. Ltd: London, 1963.

(54) Sazhin, S. S.; Abdelghaffar, W. A.; Krutitskii, P. A.; Sazhina, E. M.; Heikal, M. R. New Approaches to Numerical Modelling of Droplet Transient Heating and Evaporation. *Int. J. Heat Mass Transf.* **2005**, *48* (19–20), 4215–4228.

(55) Atkins, P. W.; De Paula, J. *Atkins’ Physical Chemistry*; Oxford University Press: Oxford, 2002.

(56) Bader, A.; Keller, P.; Hasse, C. The Influence of Non-Ideal Vapor–Liquid Equilibrium on the Evaporation of Ethanol/Iso-Octane Droplets. *Int. J. Heat Mass Transf.* **2013**, *64*, 547–558.

(57) Rogers, M. C.; Brown, G. G. *Raoult’s Law and the Equilibrium Vaporization of Hydrocarbon Mixtures*; University of Michigan, 1929.

(58) Poling, B. E.; Prausnitz, J. M.; O’Connell, J. P. *The Properties of Gases and Liquids*; McGraw-Hill: New York, 2001.

(59) Reid, R. C.; Prausnitz, J. M.; Poling, B. E. *The Properties of Gases and Liquids*, 4th ed.; McGraw-Hill: New York, 1987.

(60) Kwanchareon, P.; Luengnaruemitchai, A.; Jai-In, S. Solubility of a Diesel–Biodiesel–Ethanol Blend, Its Fuel Properties, and Its Emission Characteristics from Diesel Engine. *Fuel* **2007**, *86* (7–8), 1053–1061.

(61) Satgé de Caro, P. Interest of Combining an Additive with Diesel–Ethanol Blends for Use in Diesel Engines. *Fuel* **2001**, *80* (4), 565–574.

(62) Ni, Z.; Han, K.; Zhao, C.; Chen, H.; Pang, B. Numerical Simulation of Droplet Evaporation Characteristics of Multi-Component Acetone-Butanol-Ethanol and Diesel Blends under Different Environments. *Fuel* **2018**, *230*, 27–36.

(63) Ma, X.; Zhang, F.; Han, K.; Yang, B.; Song, G. Evaporation Characteristics of Acetone–Butanol–Ethanol and Diesel Blends Droplets at High Ambient Temperatures. *Fuel* **2015**, *160*, 43–49.

(64) Al-Esawi, N.; Al Qubeissi, M.; Sazhin, S. S.; Mwabueze, E.; Blundell, M. V. Impact of Corrected Activity Coefficient on the Estimated Droplet Heating and Evaporation. In *ICTEA: 11th International Conference on Thermal Engineering*; Doha-Qatar, 2018.

(65) Al Qubeissi, M.; Sazhin, S. S.; Elwardany, A. E. Modelling of Blended Diesel and Biodiesel Fuel Droplet Heating and Evaporation. *Fuel* **2017**, *187*, 349–355.

(66) Sazhin, S. S.; Al Qubeissi, M.; Heikal, M. R. Modelling of Biodiesel and Diesel Fuel Droplet Heating and Evaporation. In *15th International Heat Transfer Conference*; Begellhouse: Kyoto, Japan, 2014; Vol. IHTC15-8936.

(67) Bondi, A. Van Der Waals Volumes and Radii. *J. Phys. Chem.* **1964**, *68* (3), 441–451.

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2. \* Hereafter, the percentage of the substance in the mixture refers to its volume fraction unless otherwise stated. [↑](#footnote-ref-2)
3. is the volume occupied by each group in the molecule, while is the surface area occupied by each group in the molecule. The structure of the groups and the values of and in E85-diesel fuel blends are the same as those shown in Ref 36 for the ethanol-gasoline blend. Diesel fuel, however, has 5 more groups of molecules than gasoline fuel, namely, bicycloalkanes, naphthalenes, tricycloalkanes, diaromatics and phenanthrenes. The approximations of these 5 groups are discussed in Appendix A. [↑](#footnote-ref-3)