Modelling of heating and evaporation of automotive fuel droplets: recent results and unsolved problems

Sazhin, S.S. , Al Qubeissi, M. and Heikal, M.R.

MODELLING OF HEATING AND EVAPORATION OF AUTOMOTIVE FUEL DROPLETS: RECENT RESULTS AND UNSOLVED PROBLEMS

Sergei S. Sazhin[*], Mansour Al Qubeissi, Morgan R. Heikal
Sir Harry Ricardo Laboratories, Centre for Automotive Engineering,
School of Computing, Engineering and Mathematics,
University of Brighton, Brighton, BN2 4GJ, UK
[*]*Corresponding author, e-mail: S.Sazhin@brighton.ac.uk*

Abstract

The application of the discrete component model for heating and evaporation to multi-component biodiesel fuel droplets in direct injection internal combustion engines is described. This model takes into account the effects of temperature gradient, recirculation and species diffusion inside droplets. A distinctive feature of the model used in the analysis is that it is based on the analytical solutions to the transient heat transfer and species diffusion equations inside the droplets. The results of applications of the multi-dimensional quasi-discrete model to the analyses of Diesel and gasoline fuel droplet heating and evaporation are summarised. In this model, actual components of the fuel are replaced with a smaller number of components or hypothetical quasi-components. As in the original discrete component model, transient diffusion of these components/quasi-components, temperature gradient and recirculation (due to relative droplet velocities and ambient air) inside droplets are all taken into account.

Keywords: biodiesel fuel, Diesel fuel, gasoline fuel, droplets, heating, evaporation, multi-component.

1. INTRODUCTION

Fuel droplet heating and evaporation are crucial processes leading to fuel combustion in internal combustion engines [1]. The accuracy of modelling these processes is important for improving the design of these engines. This paper summarises some comparisons between the results, referring to fuel droplet evaporation times and time evolution of droplet surface temperatures and radii, predicted by the previously suggested simplified models, the recently developed version of the discrete component (DC) model and the multi-dimensional quasi-discrete (MDQD) model [2, 3]. The latter two models take into account the recirculation, temperature gradient, and diffusion of species inside the droplets, based on the Effective Thermal Conductivity and Effective Diffusivity (ETC/ED) models [1].

The main principles of the DC and MDQD models are summarised in Section 2. Some results of the application of these models to the analysis of heating and evaporation of biodiesel, Diesel and gasoline fuel droplets are presented and discussed in Sections 3–5. Some unsolved problems are summarised in Section 6.

2. MODELS

The analyses are based on the assumption that droplets are spherically symmetric. Temperature gradients and species diffusions in the liquid phase and the effect of internal recirculations due to relative velocity between ambient gas and droplets are taken into account, using the Effective Thermal Conductivity and Effective Diffusivity (ETC/ED) model. In contrast to most previously reported studies, the analyses are based on the previously obtained analytical solutions to the transient heat transfer and species diffusion equations within droplets (see [1] for further details). The effects of coupling between gas and droplets are ignored. These models are applied directly to the analysis of biodiesel fuels, containing relatively small numbers of components.

In the case of Diesel and gasoline fuels, these models were generalised to the so-called multi-dimensional quasi-discrete (MDQD) model, in which the actual composition of fuel was reduced to a much smaller number of representative components/quasi-components (C/QC). These components/quasi-components are identified from within groups of components (9 groups were identified for Diesel fuel and six groups were identified for gasoline fuel). Some components within

groups form quasi-components, while other components are considered separately. Thus, a mixture of components/quasi-components (C/QC) is formed in such a way that molar fractions of these C/QC are as close as possible. The mixtures are treated as ideal (Raoult's law is assumed to be valid). The results of calculations, using the above-described model, are compared with the predictions of simplified models based on the assumptions that liquid thermal conductivity is infinitely high (Infinite Thermal Conductivity (ITC) model) and liquid species diffusivity is infinitely fast (Infinite Diffusivity (ID) model) or infinitely slow (Single Component (SI) model).

3. BIODIESEL FUEL DROPLETS

The above-mentioned ETC/ED model was applied to 19 types of biodiesel fuel droplets. These are: Tallow Methyl Ester (TME), Lard Methyl Ester (LME), Butter Methyl Ester (BME), Coconut Methyl Ester (CME), Palm Kernel Methyl Ester (PMK), Palm Methyl Ester (PME), Safflower Methyl Ester (SFE), Peanut Methyl Ester (PTE), Cottonseed Methyl Ester (CSE), Corn Methyl Ester (CNE), Sunflower Methyl Ester (SNE), Soybean Methyl Ester (SME), Rapeseed Methyl Ester (RME), Linseed Methyl Ester (LNE), Tung Methyl Ester (TGE), Hemp-oil Methyl Ester, produced from Hemp seed oil in Ukraine (HME1), Hemp-oil Methyl Ester, produced in the European Union (HME2), Canola seed Methyl Ester (CAN) and Waste cooking-oil Methyl Ester (WME).

The time evolutions of droplet surface temperatures (T_s) and radii (R_d) for the above-mentioned 19 types of biodiesel fuels were studied [4]. It was assumed that a droplet with initial temperature and radius 350 K and 12.66 μm, respectively, is moving through air at relative velocity $U_d = 35$ m/s at temperature and pressure equal to 880 K and 30 bar respectively. An example of the time evolutions of droplet surface temperatures and radii of Butter Methyl Ester (BME) droplets is shown in Fig. 1. The following models were used in our analysis: 1) the ETC/ED model taking into account the contributions of multiple components (ME); 2) a combination of ITC and single-component models, in which all species are treated as one-component (SI); and 3) a combination of ITC and one dominant component models, in which biodiesel fuel is approximated by a single dominant component (DI). The second and third models are commonly used in the analysis of heating and evaporation of biodiesel fuel droplets.
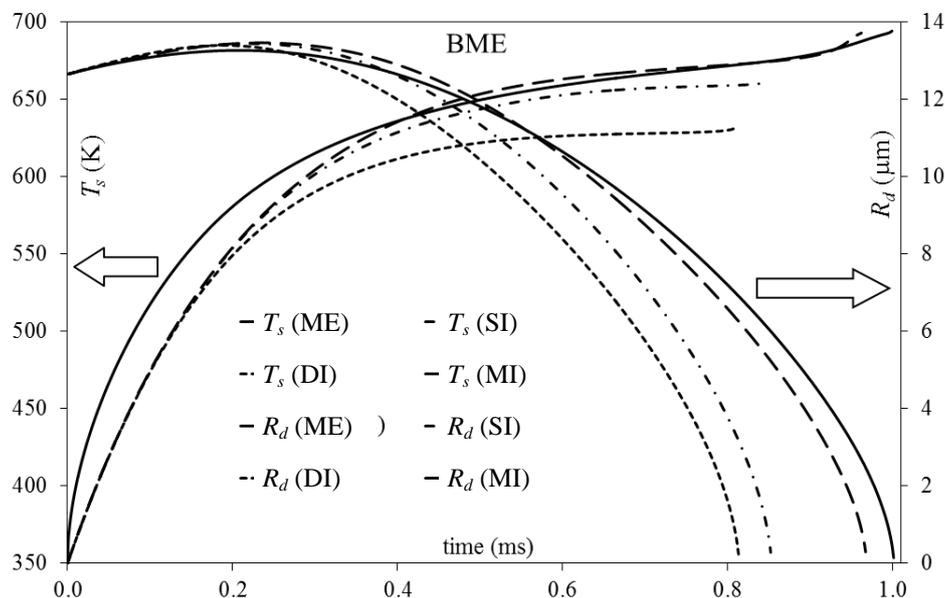

Fig. 1. The droplet surface temperatures (T_s) and radii (R_d) versus time predicted by the ME, SI, MI and DI models (see the text of the paper for the definition of these models), for a BME fuel droplet.

As one can see from Fig. 1, the errors in predictions of the droplet surface temperatures, radii and evaporation time using the conventional (single-component SI or dominant-component DI) models, compared with the predictions of the ME model, are noticeable and should not be ignored in practical engineering applications. The deviations between the predictions of these two models and the ME model indicate the importance of taking into account the diffusion of species inside droplets alongside the effects of temperature gradient within them. The errors in droplet evaporation times, predicted by

the DI and SI models compared to the ME model, were estimated for BME to be less than or equal to 18.8% and 14.9%, respectively. Also, the errors in droplet surface temperatures, predicted by the DI and SI models compared to the ME model, for BME were shown to be less than or equal to 10.4% in both cases.

As inferred from the analysis of all 19 types of biodiesel fuel droplets in conditions similar to those mentioned above, the SI model under-predicts the droplet evaporation times compared with the ME model by up to about 26%. This result does not support our earlier finding, based on the analysis of only five types of biodiesel fuel droplets in different engine conditions, which was that the deviations between the evaporation times predicted by these models do not exceed about 5.5% [2]. The evaporation times predicted by the MI model were shown to be reasonably close to those predicted by the ME model. The MI model under-predicts this time by not more than 4.3%, except for Rapeseed Methyl Ester (RME), for which this under-prediction reaches 15.1%.

4. DIESEL FUEL DROPLETS

The above-mentioned MDQD model was applied to the analysis of a typical Diesel fuel droplet. A commercial Diesel fuel conforming to standard European Union fuel (EN590) was chosen for the analysis. The detailed chemical species composition was obtained using comprehensive two-dimensional gas chromatography (GCXGC). Molar fractions of various components in this fuel are presented in Tab. 1 of [3]. The results presented in this table were simplified, taking into account that the properties of n-alkanes and iso-alkanes are rather close. This allowed us to merge n-alkanes and iso-alkanes into one group of alkanes and consider the following composition of fuel: 40.0556% alkanes, 14.8795% cycloalkanes, 7.6154% bicycloalkanes, 16.1719% alkylbenzenes, 9.1537% indanes and tetralines, 8.6773% naphthalenes, 1.5647% tricycloalkanes, 1.2240% diaromatics and 0.6577% phenanthrenes.

Assuming, following [3], that the initial droplet radius, R_{d0}, is equal to 10 μm, density, temperature and pressure of air, ρ_a, T_a, p_a, are equal to 11.9 kg/m^3, 880 K and 30 bar, respectively, the values of droplet surface temperatures and radii versus time were calculated for various approximations of Diesel fuel composition.
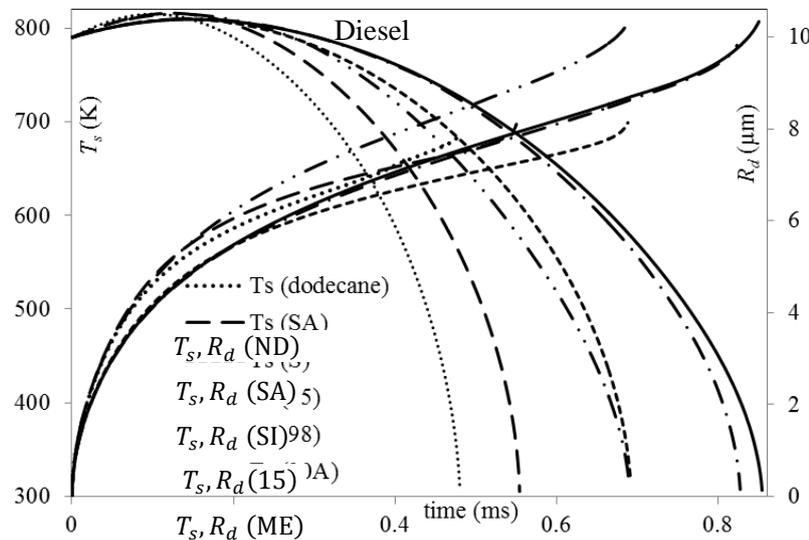

Fig. 2. The droplet surface temperatures (T_s) and radii (R_d) versus time for four approximations of Diesel fuel composition:
- the contributions of all 98 components are taken into account (curves (ME));
- the contributions of only 20 alkane components are taken into account (curves (20A));
- the contributions of all 98 components are approximated by 9 C/QC, 6 quasi-components (corresponding to the first 6 groups) and 3 components (tricycloalkane, diaromatic and phenanthrene), without taking into account the diffusion among them (curves (SI));
- the contributions of only 20 alkanes are taken into account and these are treated as a single component (curves (SA));
- the contributions of all 98 components are approximated by 15 C/QC (curves (15)); and
- the contributions of all 98 components are approximated by n-dodecane (curves (ND)).

183

In Fig. 2 these plots are shown for six cases: the contributions of all 98 components are taken into account (indicated as (ME)); the contributions of only 20 alkane components are taken into account (indicated as (20A)); the contribution of all 98 components is approximated by six quasi-components (corresponding to the first six groups mentioned above) and three components (tricycloalkane, diaromatic and phenanthrene) without taking into account the diffusion between them so that their mass fractions remain equal to the initial mass fractions and they behave like a single quasi-component (indicated as (SI)); the contributions of only 20 alkane components are taken into account and these are approximated by a single quasi-component with the average value of the carbon number ($C_{14.763054}H_{31.526108}$, indicated as (SA)); the contribution of all 98 components is approximated by 15 C/QC (indicated as (15)); and Diesel fuel is replaced by n-dodecane (indicated as (ND)). In the cases when only the contribution of alkanes was taken into account, the mass fractions of the components were recalculated to ensure that the total mass fractions of all alkanes were equal to 1.

As follows from Fig. 2, the approximation of 98 actual components with a single quasi-component leads to a noticeable under-estimation of the droplet surface temperatures, and an under-estimation of the evaporation time by about 20%. In the case when Diesel fuel is approximated with 20 alkane components, the predicted droplet surface temperatures appeared to be higher by about 11% and the evaporation time shorter by about 27% than in the case of approximation of Diesel fuel with 98 components. This means that the approximation of Diesel fuel with alkanes, a widely used assumption in the modelling of Diesel fuels (see [1] and the references therein), leads to results which are less accurate, compared with the approximation of Diesel fuel by a single quasi-component. The approximation of Diesel fuel with a single alkane quasi-component $C_{14.763054}H_{31.526108}$ leads to under-prediction of the evaporation time by about 40% which is not acceptable even for qualitative analysis of the process. The replacement of Diesel fuel with n-dodecane, which is widely practiced in many engineering applications, leads to under-prediction of the evaporation time by about 45%; while the approximation of Diesel fuel with 15 C/QC, using the MDQD model, leads to only about 2.5% error in the evaporation time. This shows the benefit of using the MDQD model in comparison to other approaches.

5. GASOLINE FUEL DROPLETS

The above-mentioned MDQD model was also applied to the analysis of a typical gasoline fuel droplet. A typical gasoline fuel composition, inferred from [5], was used in our analysis. The components with identical chemical formulae and close thermodynamic and transport properties were replaced with characteristic components in the groups, leading to the approximation of gasoline fuel with 20 components. Using the multi-dimensional quasi-discrete (MDQD) model, as in the case of Diesel fuel, 20 actual components of the fuel were replaced with a smaller number of components/quasi-components (C/QC). Transient diffusion of these C/QC in the liquid phase, temperature gradient and recirculation inside droplets were all taken into account. In contrast to the case of Diesel fuel, where n-alkanes and iso-alkanes were merged into one group of alkanes, separate contributions of these two groups were taken into account in the analysis of gasoline fuel droplets.

The following set of in-house experimentally measured parameters was used in the analysis. The mean radius of droplets at the early stage of evaporation was taken to be equal to 12 µm, their relative velocities and initial temperatures were assumed equal to $U_d = 24$ m/s and $T_d = 296$ K respectively, ambient air pressure and temperature were assumed equal to $p_a = 9$ bar and $T_a = 545$ K, respectively.

The plots of the droplet surface temperatures T_s and radii R_d versus time are presented in Fig. 3. Five cases are shown: (1) the contributions of all 20 components are taken into account using the ETC/ED model (indicated as (ME)); (2) the contributions of 20 components are taken into account using the ITC/ID model (indicated as (MI)); (3) the thermodynamic and transport properties of 20 components are averaged to form a single component and temperature gradient is ignored (ITC model) (indicated as (SI)); (4) the ITC model in which gasoline fuel is approximated with iso-octane (2,2,4-trimethylpentane, indicated as (IO)); and (5), the model in which 20 components are approximated by 6 QC (2 QC of n-alkanes, 2 QC of iso-alkanes, and 2 QC of aromatics) (indicated as (6)).
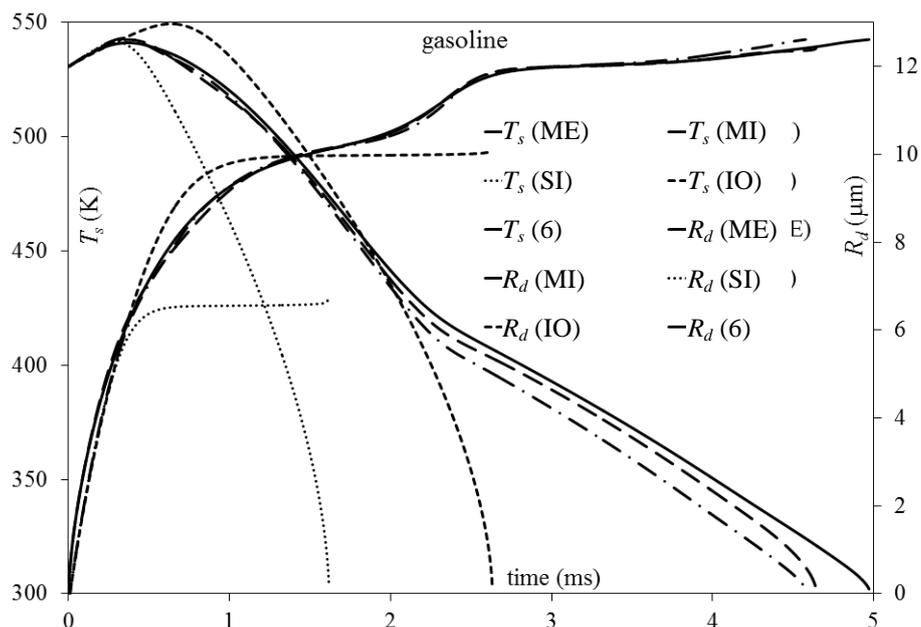
Fig. 3. The droplet surface temperatures (T_s) and radii (R_d) versus time for the cases when:
   (1) the contributions of all 20 components are taken into account using the ETC/ED model (ME);
   (2) the contributions of 20 components are taken into account using the ITC/ID model (MI);
   (3) the 20 components are approximated by a single component with average thermodynamic and transport properties in combination with the ITC model (SI);
   (4) fuel is approximated by iso-octane in combination with the ITC model (IO);
   (5) the 20 components are approximated by 6 C/QC;
   (6) a droplet with initial radius 12 µm and initial homogeneous temperature 296 K is assumed to be moving with relative velocity 24 m/s in air at pressure and temperature equal to 0.9 MPa and 545 K, respectively.

As one can see from Fig. 3, the errors in droplet surface temperatures and evaporation times, predicted by the SI model, are 13.6% and 67.5%, respectively. These errors were reduced to 6.3% and 47.1%, when the IO model was used, to 4.8% and 8% when the MI model was used, and were further reduced to 0.84% and 6.6%, when gasoline fuel was approximated to 6 QC using the MDQD model. Although the accuracy of the MI and IO models might be acceptable in some limited engineering applications, these models cannot describe adequately the underlying physics of the processes inside droplets (heat conduction and species diffusion).

As can be seen from Fig. 3, the approximation of the actual composition of gasoline fuel by 6 C/QC, using the MDQD model, leads to errors in estimated droplet surface temperatures and evaporation times of about 0.8% and 6.6% respectively, which can be tolerated in many engineering applications. Also, it was shown that the application of the latter model leads to about 70% reduction in CPU time compared to the model taking into account all 20 components of gasoline fuel.

6. UNSOLVED PROBLEMS

Although the results described above show noticeable progress in the development of the models of automotive fuel droplet heating and evaporation, many important problems in this area are still not resolved. The focus of this section will be on some of these unsolved problems. The selection of these problems is rather subjective, and has been largely motivated by the authors' personal research interests.

The models discussed above are applicable only to spherical droplets, while the shapes of most of the droplets observed in internal combustion engines are far from spherical [6]. The application of analytical models for spherical droplets to the case of moving droplets has been based on the assumption that the ETC/ED model is valid. The validity of this model has been investigated based on the direct comparison of the predictions of this model and the prediction of a more general vortex model for a limited range of parameters (see this comparison for the ETC model presented in [7]). The applicability of the model outside this range is far from obvious.

As demonstrated in a number of our recent papers (e.g., [8]), even in the simple case of droplets moving in tandem the effect of interaction between droplets on their heating and evaporation cannot be

ignored when the distance parameter (ratio of the distance between droplets and their diameter) is less than about 10. Various semi-empirical formulas taking into account these interactions have been suggested. However, in realistic internal combustion engines the mutual positions of moving droplets are expected to be quite complex. Also, the number of droplets affecting any particular droplet in a dense spray can be rather large. It is not clear how this complex interaction between droplets can be taken into account when modelling individual droplet heating and evaporation.

ACKNOWLEDGEMENTS

REFERENCES

[1] Sazhin S S. Droplets and Sprays. Springer, London. 2014.

[2] Sazhin S S, Al Qubeissi M, Kolodnytska R, Elwardany A E, Nasiri R, Heikal M R. Modelling of biodiesel fuel droplet heating and evaporation. Fuel 115 (2014), p. 559–572.

[3] 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 129 (2014), p. 238–266.

[4] Al Qubeissi M, Sazhin S S, Crua C, Heikal M R. Modelling of heating and evaporation of biodiesel fuel droplets. World Academy of Science, Engineering and Technology, International Science Index 97, International Journal of Mechanical, Aerospace, Industrial and Mechatronics Engineering 9 (2015), p. 46-49.

[5] Sarathy S M, Kukkadapu G, Mehl M, Wang W, Javed T, Park S, Oehlschlaegerd M A, Farooq A, Pitz W J, Sungb C-J. Ignition of alkane-rich FACE gasoline fuels and their surrogate mixtures. Proceedings of the Combustion Institute 35 (2015), p. 249–257.

[6] Crua C, Shoba T, Heikal M, Gold M, Higham C. High-speed microscopic imaging of the initial stage of Diesel spray formation and primary breakup. SAE Report (2010), 2010-01-2247.

[7] Abramzon B, Sazhin S S. Convective vaporization of a fuel droplet with thermal radiation absorption. Fuel 85 (2006), p. 32–46.

[8] 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. International Journal of Thermal Sciences 50 (2011), p. 1164–1180.