

## Models for automotive fuel droplets heating and evaporation

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### Abstract

The paper presents recent approaches to the modelling of heating and evaporation of automotive fuel droplets with application to biodiesel, diesel, gasoline, and blended fuels in conditions representative of internal combustion engines. The evolutions of droplet radii and temperatures for gasoline, diesel, and a broad range of biodiesel fuels and their selective diesel fuel blends have been predicted using the Discrete Component model (DCM). These mixtures combine up to 112 components of hydrocarbons and methyl esters. The results are compared with the predictions of the case when blended diesel-biodiesel fuel are represented by pure fossil and biodiesel fuels. In contrast to previous studies, it is shown that droplet evaporation time and surface temperature predicted for 100% biodiesel (B100) are not always close to those predicted for pure diesel fuel. Also, the previously introduced Multi-Dimensional Quasi-Discrete model and its application to these fuels and their mixtures are discussed. The previous application of this model has resulted in up to 96% reduction in CPU time compared to the case when all fuel components are considered using the DCM.

### Keywords

Biodiesel, Diesel, Fuel droplet, Fuel blends, Gasoline

### Introduction

There have been several attempts to simulate fuel droplets heating and evaporation. These have been either based on the analysis of individual components, the discrete component model (DCM) [1–3], or on the probabilistic analysis of a large number of components (the continuous thermodynamics [4–6] and the distillation curve ([7–9] models). In most studies, several simplifying assumptions have been made, e.g. species inside droplets mix infinitely quickly (infinite diffusivity (ID) model) or do not mix at all (the single component (SC) model). Also, the temperature gradients inside droplets have been ignored in most cases with the assumption that the liquid thermal conductivity is infinitely large (infinite thermal conductivity (ITC) model). This paper will present our recent approaches to address these gaps in literature.

Based on recent research findings (e.g. [3,10–13]), the drawbacks in modelling fuel droplets heating and evaporation processes (computationally expensive models, ignoring temperature gradient and transient species diffusion) are partially addressed using the MDQD model. 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 DCM and the multi-dimensional quasi-discrete model (MDQDM) [14–16]. 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.

In the following section (Models), the main principles of the DCM and MDQDM are summarised. The results of using these models for the analysis of heating and evaporation of biodiesel, diesel and gasoline fuel droplets, and their blends are reviewed in the Sections: Biodiesel fuel droplets, Diesel Fuel Droplets, Gasoline fuel droplets, and Blended diesel-biodiesel fuel droplets, respectively. The impact of in-cylinder conditions on these fuel droplets' lifetimes are presented in the Section of 'Impact of in-cylinder conditions'. The results are summarised in the Section of Conclusions.

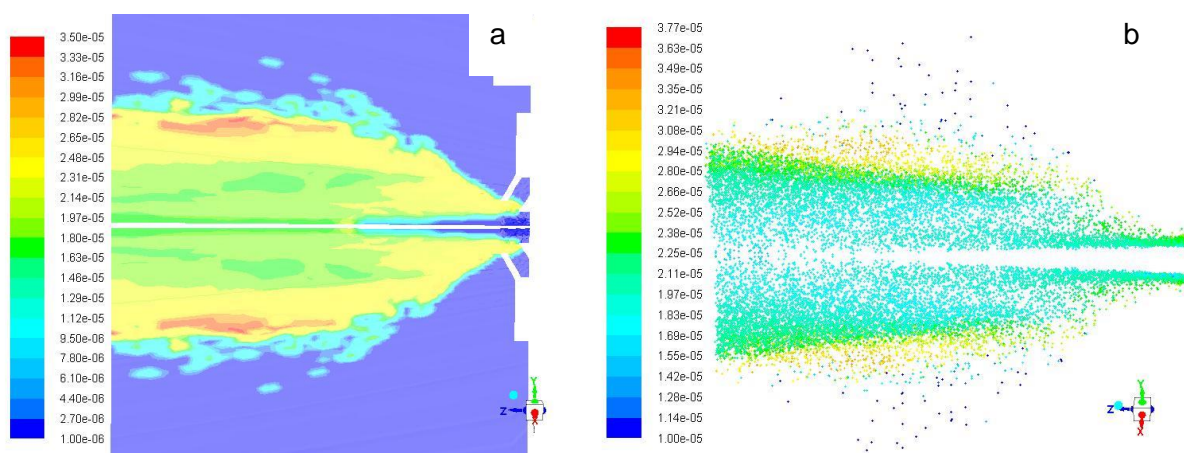
### Models

In the case of small number of components (e.g. biodiesel fuels), DCM approach (described in [2,10,13,17]) is easily implemented, where the number of components (up to 14 components) are relatively small. In the DCM analyses, we assume that droplets are spherically symmetric but temperature gradients and species diffusions in the liquid phase and the effect of internal recirculation due to relative velocity between ambient gas and droplets are all accounted for, using the Effective Thermal Conductivity and Effective Diffusivity (ETC/ED) models.

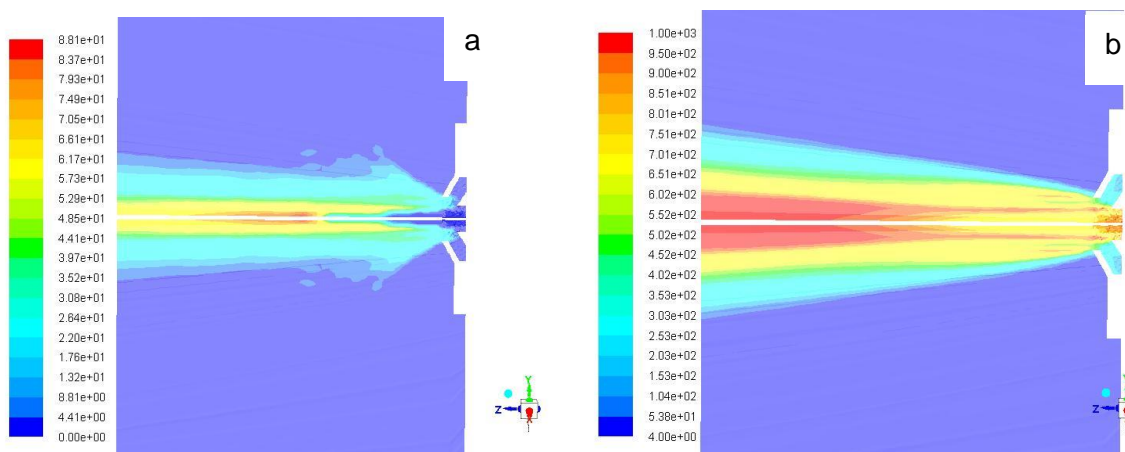
In the cases of diesel, gasoline, and diesel-biodiesel blended fuels, the MDQDM approach, in which the actual composition of fuel is reduced to a much smaller number of representative components/quasi-components (C/QC), is used. These components/quasi-components are formed within groups of components (e.g. 9 groups of diesel fuel species, 6 groups of gasoline fuel species, and 4 groups of FAME (Fatty Acid Methyl Ester) biodiesel fuel species). Some components within groups form quasi-components, while other components are considered separately described as characteristic components. 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 (for further details about this approach, see [12,14–16]).

We assume droplets with several initial homogeneous temperatures and radii within the ranges of 300-360 K and 10-15  $\mu\text{m}$ , respectively, are moving through air at relative velocities of  $U_{cl}$ = 0-35 m/s, under ambient temperatures and pressures of 500-800 K and 5-50 bar, respectively.

The verification of the selected droplet SMD and velocities have been made using ANSYS-Fluent 17.2 simulation; typical examples of which are shown in Figures 1 and 2 using realizable k- $\epsilon$  model and air-blast atomizer for injection.



**Figure 1.** SMD and droplets distribution of a diesel fuel spray in conditions averaged from those presented in this paper, showing the contour gradient of SMD (a) and space distribution (b), produced using ANSYS-Fluent 17.2.

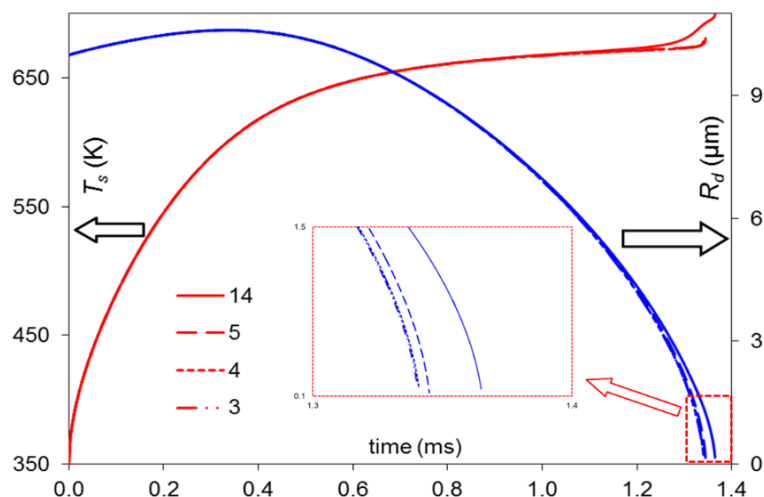


**Figure 2.** Droplets velocity gradient (a) and turbulence intensity (b) of diesel fuel spray in conditions averaged from those presented in this paper, produced using ANSYS-Fluent 17.2.

### Biodiesel fuel droplets

The interest in biodiesel fuels has been mainly stimulated by depletion of fossil fuels and the need to reduce emissions that contribute toward climate change [18]. Biodiesel fuel can be blended with fossil fuels and used in many different concentrations. For instance, a mixture of 95% diesel and 5% biodiesel (B5) fuel can be called diesel fuel, with no separate labelling required at the pump [19]. Hence, it is essential to investigate the validity of this assumption based on estimated droplets lifetimes of both, fossil and its FAME biodiesel blended, fuels.

Both, the DCM and MDQDM, approaches are applied to 22 types of FAME biodiesel fuel droplets. These methyl esters are: tallow (TME), lard (LME), butter (BME), coconut (CME), palm kernel (PMK), palm (PME), safflower (SFE), peanut (PTE), cottonseed (CSE), corn (CNE), sunflower (SNE), soybean (SME), rapeseed (RME), linseed (LNE), tung (TGE), hemp-oil, produced from hemp seed oil in the Ukraine (HME1), hemp-oil, produced in European Union (HME2), canola (CAN), waste cooking-oil (WCO), yellow grease oil (YME), camelina (CML), and jatropha (JME). A typical example of applying the MDQDM to FAME biodiesel fuel is shown for waste cooking oil (WCO) methyl esters in Figure 3; in which 14 methyl esters of the fuel are reduced to 5, 4 and 3 C/QC [20].

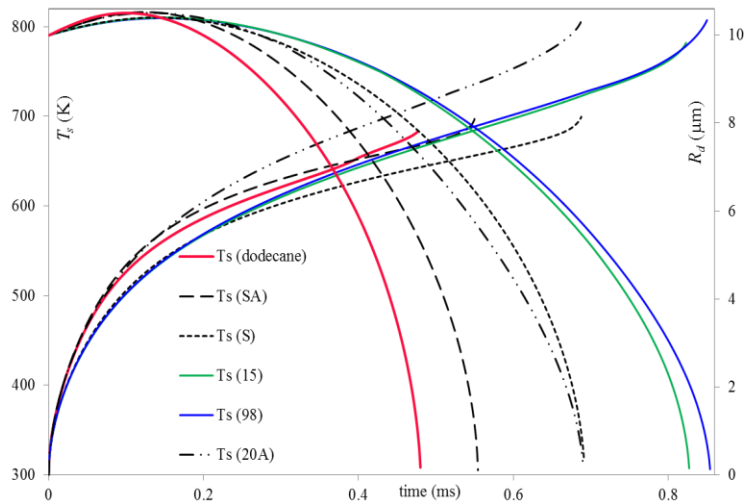


**Figure 3.** The plots of droplet surface temperatures ( $T_s$ ) and radii ( $R_d$ ) versus time for various WCO fuel using the MDQDM. The initial droplet radius and temperature were 10  $\mu\text{m}$  and 350 K respectively. The ambient gas temperature and pressure were 800 K and 30 bar respectively. The droplet was moving at constant velocity 10 m/s in still air.

As can be seen from Figure 3, replacing the full composition of WCO methyl esters with 5, 4 and 3 C/QC produces almost identical plots for the evolutions of  $T_s$  and  $R_d$ . The predicted errors in estimating  $T_s$  evolutions of these C/QC approximations compared to those for 14 components are less than about 2%, while the same errors for the prediction of droplet lifetimes are less than about 1.8%. Hence, there is no noticeable reduction in the accuracy of predicting the droplet lifetimes or surface temperatures due to the implementation of the MDQD model. At the same time, using the MDQD model improves computational efficiency significantly. For B100 WCO, the MDQD model resulted in a reduction of up to 96% in computational time compared with the case when the original 14 components are considered using the DCM.

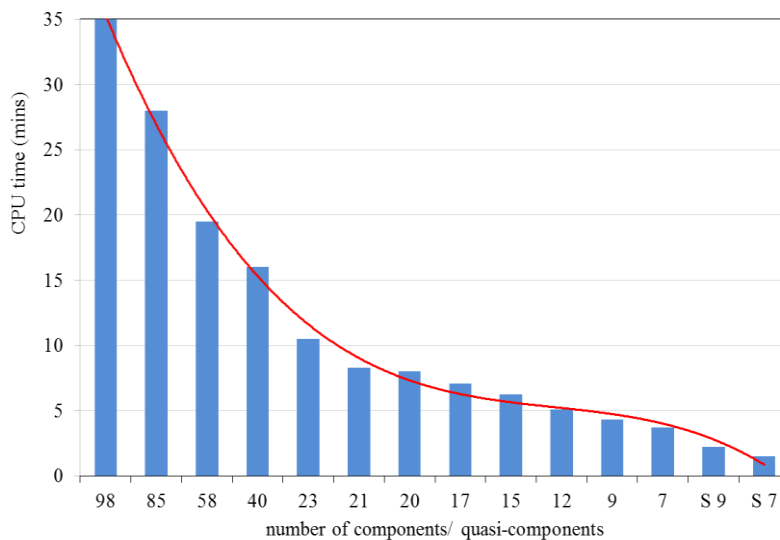
### Diesel fuel droplets

The plots of typical evolutions of droplet surface temperatures  $T_s$  and radii  $R_d$  versus time for diesel fuel droplet as predicted by the DCM and MDQDM approaches, accounting for the contributions of all 98 components, are shown in Figure 4. The plots in this figure illustrate 4 cases as presented in [14,15]: the contributions of all 98 components are taken into account using the DCM (labelled as “(98)”; the contributions of only 20 alkane components are taken into account using the ID/ITC model (following the approximation used in [21,22]) (labelled “(20A)”; the contributions of all 98 components are approximated by 15 C/QC using the MDQDM; and the contribution of only n-dodecane is taken into account using the SC model. As can be seen from this figure, the approximation of Diesel fuel by classical approaches, such as 20 alkane components, SC (e.g. n-dodecane), ITC and ID models, lead to under-estimation of droplet evaporation time by up to 50%, which are not acceptable in many engineering applications. At the same time, the approximation of 98 components of Diesel fuel by 15 C/QC leads to acceptable prediction of less than 3% error compared to the droplet lifetime predicted by the DCM, which can be acceptable in most applications.



**Figure 4.** The plots of  $T_s$  and  $R_d$  versus time for a diesel fuel droplets, predicted using the MDQDM (indicated as 15), SC/ETC/ED model (indicated as S, SA and dodecane), ITC/ID model (indicated as 20A), and DCM (indicated as 98). The droplet of  $12.66 \mu\text{m}$  initial radius and  $360 \text{ K}$  temperature is moving at  $10\text{m/s}$  in still air of pressure and temperature equal to  $32 \text{ bar}$  and  $700 \text{ K}$ , respectively.

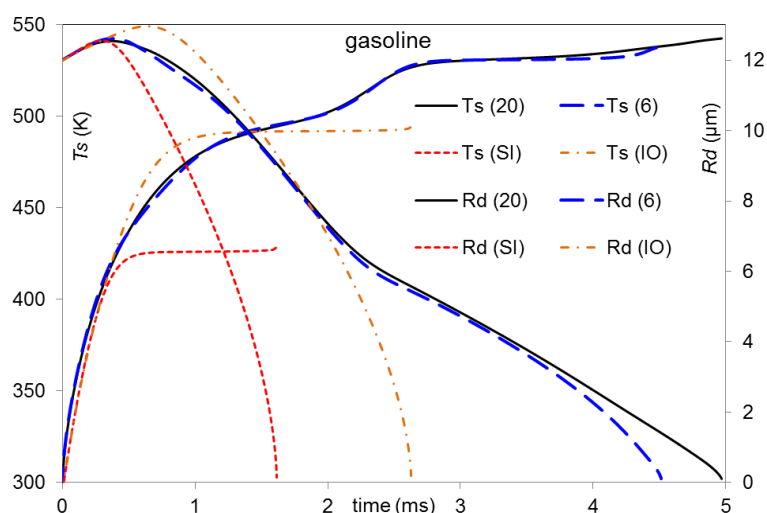
Using the MDQD model (shown in Figure 4) has contributed to reducing the CPU time to 1/6th compared with the model considering the contributions of all 98 components, as shown in Figure 5.



**Figure 5.** The plot of CPU time required for calculations of stationary diesel fuel droplet heating and evaporation for Intel Xeon (core duo) E8400, 2 GHz and 3 GB RAM for  $1 \mu\text{s}$  time-step.

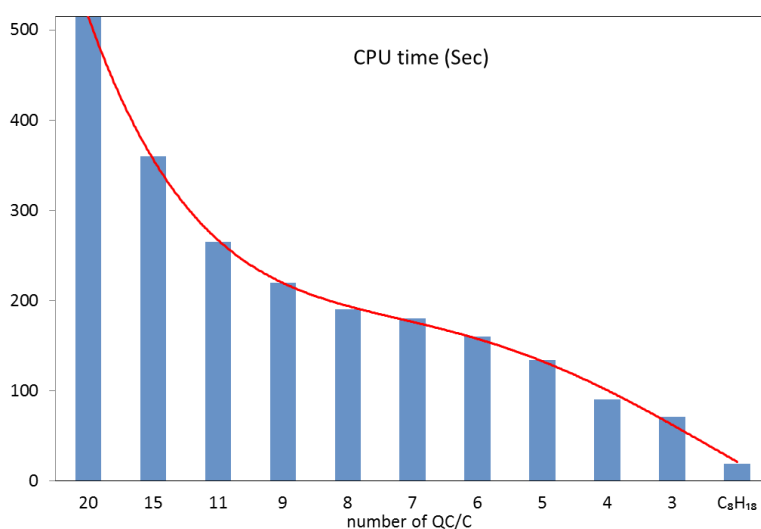
### Gasoline fuel droplets

The evolutions of the droplet surface temperatures  $T_s$  and radii  $R_d$  versus time for gasoline FACE C fuel are presented in Figure 6. In this figure, four cases have been examined [16]: (1) the contributions of all 20 components are taken into account using the DCM (indicated as ME); (2) the contributions of 20 components are taken into account, but represented by 6 C/QC using the MDQDM (indicated as 6); (3) the thermodynamic and transport properties of 20 components are averaged to form a single component and temperature gradient is ignored (SC and ITC models) (indicated as SI); and (4) the ITC model in which gasoline fuel is approximated with iso-octane (indicated as IO) is used. As one can see from this figure, the errors in droplet lifetimes predicted by the classical approaches, such as SI, IO, or MI models, are up to about 68%, which cannot be tolerated in any engineering application. However, the errors in droplet surface temperatures and evaporation times predicted by the MDQDM using 6 QC/C are 0.8% and 6.6%, respectively, which can be tolerated in many applications.



**Figure 6.** The plots of  $T_s$  and  $R_d$  versus time for gasoline fuel droplets, predicted using the MDQDM (indicated as 6), SC/IT/ID model (indicated as SI), SC/ET/ED model (indicated as IO), and DCM (indicated as 20). The droplet with initial radius 12  $\mu\text{m}$  and initial temperature 296 K is assumed to be moving with relative velocity 24 m/s in air. Ambient pressure and temperature are equal to 0.9 MPa and 545 K respectively.

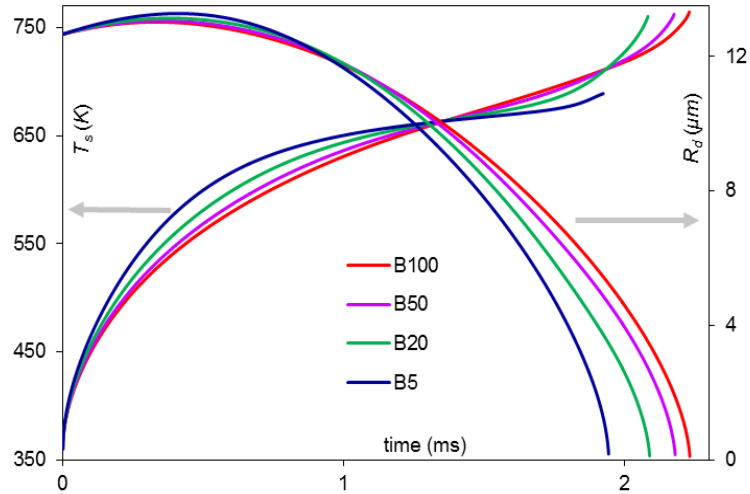
The use of the MDQDM (shown in Figure 6) has contributed to significant increase of CPU efficiency by reducing 70% of the CPU time spent to run the DCM for the same fuel (See Figure 7).



**Figure 7.** The plot of CPU time required for calculations of stationary gasoline fuel droplet heating and evaporation for Intel Xeon (core duo) E8400, 2 GHz and 3 GB RAM for 1  $\mu\text{s}$  time-step.

### Blended diesel-biodiesel fuel droplets

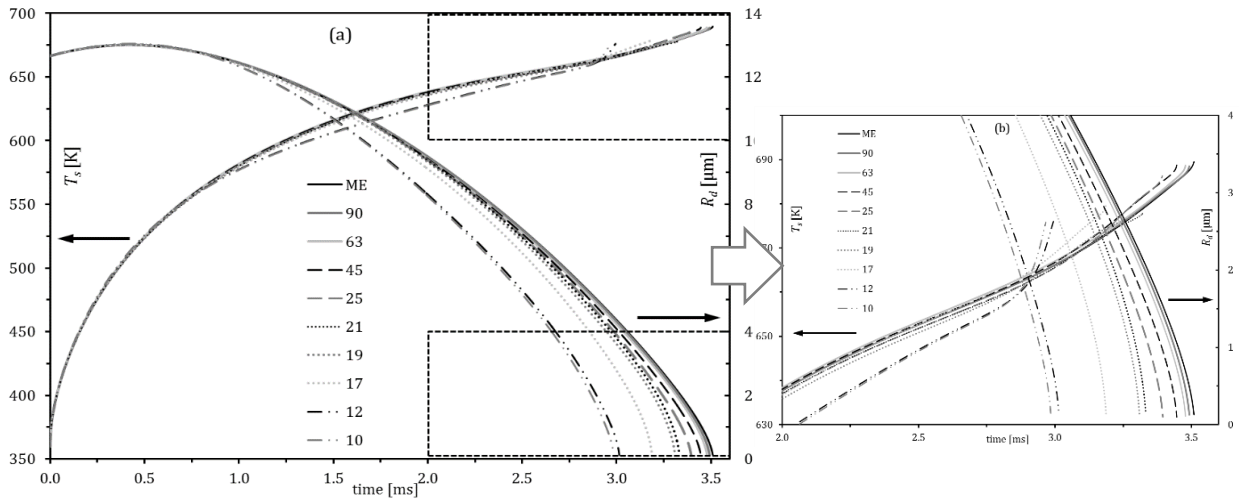
The blended fuel droplet heating and evaporation for diesel-biodiesel fuels and their blends, taking into account the contributions of all (up to 114) components of hydrocarbons and methyl esters have been investigated [12]. Both, DCM and MDQDM, approaches are considered. As inferred from previous analyses, the blends of all 22 types of biodiesel fuel with commercial used diesel fuel in certain conditions like aforementioned are tested (see Figure 8).



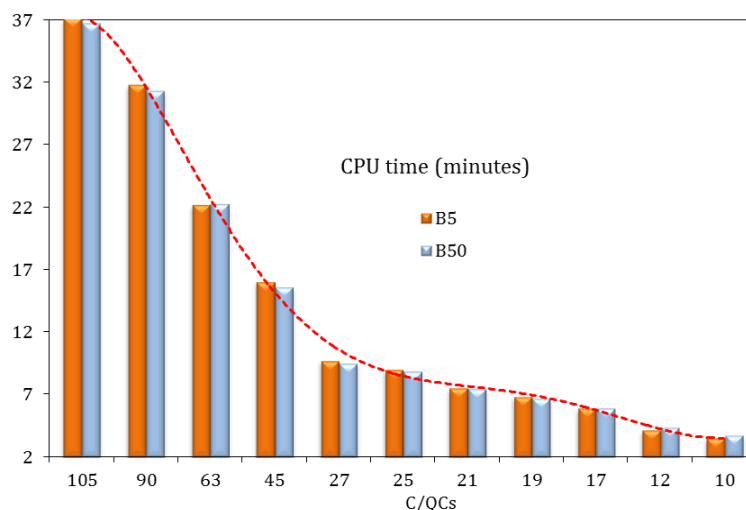
**Figure 8.** The plots of  $T_s$  and  $R_d$  versus time predicted by the DCM, for a diesel-BME blended fuel droplets moving at 10 m/s, with 12.66  $\mu\text{m}$  initial radius, 360 K initial temperature, and ambient pressure and temperature of 30 bar and 800 K, respectively.

A typical example of the time evolutions of droplet surface temperatures  $T_s$  and radii  $R_d$  of diesel-biodiesel blended fuel droplets, using DCM, was given for Butter Methyl Ester (BME) droplets in Figure 8. In this figure, four mixtures of diesel-biodiesel fuels were shown; B100 (pure biodiesel fuel), B50 (50% biodiesel and 50% diesel fuels), B20 (20% biodiesel and 80% diesel fuels) and B5 (5% biodiesel and 95% diesel fuels).

A typical example of the evolutions of  $T_s$  and  $R_d$  over time for a B5 diesel-biodiesel fuel blend (5% biodiesel and 95% diesel) droplet is shown in Figure 9. The approximations of the blended fuel of 105 hydrocarbons and methyl esters with 25 C/QCs lead to underestimation of droplet lifetime by less than 3.2%. This underestimation increases to arrange between 4%-15% for a selection range between 21 to 10 C/QCs, respectively. The errors in predicted droplet surface temperatures for all MDQDM approximations were up to 2%. Using the MDQDM for this analysis has made significant contribution to the CPU efficiency of the code (See Figure 10).



**Figure 9.** The plots of  $T_s$  and  $R_d$  versus time for various Diesel/SME blends, using the DCM and MDQDM approaches. The initial droplet radius is taken equal to 12.66  $\mu\text{m}$ , its axial velocity in still air (assumed constant) and initial temperature are assumed equal to  $U_{\text{drop}} = 10$  m/s and  $T_d = 360$  K, respectively; ambient air (gas) pressure and temperature are assumed equal to  $p_g = 32$  bar and  $T_g = 700$  K, respectively. The data and compositions of these approximations are inferred from [12].



**Figure 10.** The plot of CPU time required for calculations of droplet heating and evaporation versus the number of C/QCs for B5 and B50 fuel droplets, using the same parameters as in Figure 8. The specifications of the workstation used were: Z210, Intel core, 64-bit, 3.10 GHz and 8 GB RAM.

An example of the impact of using the MDQDM approach on the computational costs among these several approximations is illustrated in Figure 10. As can be seen from this figure, approximating 105 components of the blended fuel with 17 C/QCs reduces the required CPU time by more than 83% compared with the DCM approach considering the contributions of all 105 components. Also, it has been found that the droplet lifetime predicted for 17 C/QC is about 4% for B50, and 9% for B5, less than that predicted by the model considering the contributions of full blended fuel composition (all 105 components). Such an option can ensure a good compromise between CPU efficiency of the model and its accuracy when small errors in predicted droplet evaporation times can be tolerated for commonly used fuel blends.

## Conclusions

The modelling of the heating and evaporation of multi-component biodiesel, diesel, gasoline, and blended diesel-biodiesel fuel droplets has been performed using the Discrete Component model (DCM) and the Multi-Dimensional Quasi-Discrete Model (MDQDM). It can be concluded that ignoring the effects of species diffusion, temperature gradient and recirculation inside droplets can lead to noticeable errors in the predictions of droplet surface temperatures and evaporation times.

The influence of increasing the fraction of biodiesel in the diesel-biodiesel mixture on droplet surface temperature and evaporation time is shown to be noticeable, and it needs to be accounted for in engineering modelling. Smaller fractions of biodiesel fuel (up to 5%) have very small effects on the evolutions of droplet surface temperatures ( $T_s$ ) and radii ( $R_d$ ).

The application of the models to diesel, gasoline, and several types of biodiesel fuel is investigated. It is shown that the errors in the estimated  $T_s$  and  $R_d$  for selected number of components/quasi-components of fuels, using the MDQD model, are negligible compared to those predicted by the model considering the contributions of all components of these fuels (i.e. using the DCM). For instance, replacing the full composition of WCO methyl esters with 5, 4 and 3 C/QC produces almost identical plots for the evolutions of  $T_s$  and  $R_d$ . It can be concluded that the predictions of the MDQDM are very close to those of the DCM. At the same time, using the MDQDM has resulted in a reduction of up to 96% in computational time compared to the cases when the original full compositions of fuels are considered using the DCM.

## Acknowledgment

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## Nomenclature

B#	­% biodiesel/Diesel fraction	CML	camelina methyl ester
BME	butter methyl ester	CNE	corn methyl ester
C/QC	components/quasi-components	CPU	central processing unit
CAN	canola methyl ester	CSE	cottonseed methyl ester
CME	coconut methyl ester	DCM	discrete component model

ED	effective diffusivity	SNE	sunflower methyl ester
ETC	effective thermal conductivity	TGE	tung methyl ester
FAME	fatty acid methyl ester	TME	tallow methyl ester
HME1	hemp-oil, Ukrainian hemp seed oil	WCO	waste cooking oil
HME2	hemp-oil, produced in the European Union	YME	yellow grass oil methyl ester
ID	infinite diffusivity		
ITC	infinite thermal conductivity	<b>Symbols</b>	
JME	jatropha methyl ester	$p$	gas pressure
LME	lard methyl ester	$R$	radius
LNE	linseed methyl ester	$T$	temperature
MDQDM	multi-dimensional-quasi-discrete model	$U$	velocity
PME	palm methyl ester		
PMK	palm kernel methyl ester	<b>Subscripts</b>	
PTE	peanut methyl ester	$g$	gas
RME	rapeseed methyl ester	$d$	droplet
SC	single component	$s$	droplet surface
SFE	safflower methyl ester		
SME	soybean methyl ester		

## References

- [1] Ra, Y., and Reitz, R. D., 2009, *Int. J. Multiph. Flow*, **35**(2), pp. 101–117.
- [2] Sazhin, S. S., Al Qubeissi, M., Kolodnytska, R., Elwardany, A. E., Nasiri, R., and Heikal, M. R., 2014, *Fuel*, **115**, pp. 559–572.
- [3] Al Qubeissi, M., 2015, *Heating and Evaporation of Multi-Component Fuel Droplets*, WiSa, Stuttgart.
- [4] Zhu, G.-S., and Reitz, R. D., 2002, *Int. J. Heat Mass Transf.*, **45**(3), pp. 495–507.
- [5] Laurent, C., Lavergne, G., and Villedieu, P., 2009, *Comptes Rendus Mécanique*, **337**(6–7), pp. 449–457.
- [6] Grote, M., Lucka, K., and Köhne, H., 2010, *VECCOMAS CFD*, Lisbon, Portugal.
- [7] Burger, M., Schmehl, R., Prommersberger, K., Schäfer, O., Koch, R., and Wittig, S., 2003, *Int. J. Heat Mass Transf.*, **46**(23), pp. 4403–4412.
- [8] Smith, B. L., and Bruno, T. J., 2006, *Int. J. Thermophys.*, **27**(5), pp. 1419–1434.
- [9] Aleiferis, P. G., and van Romunde, Z. R., 2013, *Fuel*, **105**, pp. 143–168.
- [10] Sazhin, S. S., 2014, *Droplets and Sprays*, Springer, London.
- [11] Al Qubeissi, M., Sazhin, S. S., Crua, C., Turner, J., and Heikal, M. R., 2015, *Fuel*, **154**, pp. 308–318.
- [12] Al Qubeissi, M., Sazhin, S. S., and Elwardany, A. E., 2017, *Fuel*, **187**, pp. 349–355.
- [13] Sazhin, S. S., 2017, *Fuel*, **196**, pp. 69–101.
- [14] Sazhin, S. S., Al Qubeissi, M., Nasiri, R., Gun'ko, V. M., Elwardany, A. E., Lemoine, F., Grisch, F., and Heikal, M. R., 2014, *Fuel*, **129**, pp. 238–266.
- [15] Al Qubeissi, M., Sazhin, S. S., de Sercey, G., and Crua, C., 2014, *26th European Conference on Liquid Atomization and Spray Systems*, University of Bremen, Bremen, Germany.
- [16] Al Qubeissi, M., Sazhin, S. S., Turner, J., Begg, S., Crua, C., and Heikal, M. R., 2015, *Fuel*, **159**, pp. 373–384.
- [17] Al Qubeissi, M., Kolodnytska, R., and Sazhin, S. S., 2013, *25th European Conference on Liquid Atomization and Spray Systems*, Crete, Greece.
- [18] Lapuerta, M., Armas, O., and Rodriguezfernandez, J., 2008, *Prog. Energy Combust. Sci.*, **34**(2), pp. 198–223.
- [19] US Department of Energy: Energy Efficiency and Renewable Energy, [http://www.afdc.energy.gov/fuels/biodiesel\\_blends.html](http://www.afdc.energy.gov/fuels/biodiesel_blends.html). [Accessed: 13-Mar-2017].
- [20] Al Qubeissi, M., and Sazhin, S. S., 2016, *26th European Conference on Liquid Atomization and Spray Systems*, Brighton, UK, p. 179.
- [21] Elwardany, A. E., and Sazhin, S. S., 2012, *Fuel*, **97**, pp. 685–694.
- [22] Sazhin, S. S., Elwardany, A. E., Sazhina, E. M., and Heikal, M. R., 2011, *Int. J. Heat Mass Transf.*, **54**(19–20), pp. 4325–4332.