Modelling of Heating and Evaporation of Gasoline Fuel Droplets: A Comparative Analysis of Approximations

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Abstract

Modelling of gasoline fuel droplet heating and evaporation processes is investigated using several approximations of this fuel. These are quasi-components used in the quasi-discrete model and the approximations of these quasi-components (Surrogate I (molar fractions: 83.0% *n*-C_6H_{14} + 15.6% *n*-$C_{10}H_{22}$ + 1.4% *n*-$C_{14}H_{30}$) and Surrogate II (molar fractions: 83.0% *n*-C_7H_{16} + 15.6% *n*-$C_{11}H_{24}$ + 1.4% *n*-$C_{15}H_{32}$))**.** Also, we have used Surrogate A (molar fractions: 56% *n*-C_7H_{16} + 28% *iso*-C_8H_{18} + 17% C_7H_8) and Surrogate B (molar fractions: 63% *n*-C_7H_{16} + 20% *iso*-C_8H_{18}+ 17% C_7H_8), originally introduced based on the closeness of the ignition delay of surrogates to that of gasoline fuel. The predictions of droplet radii and temperatures based on three quasi-components and their approximations (Surrogates I and II) are shown to be much more accurate than the predictions using Surrogates A and B.

1. Introduction

Gasoline fuel is widely used in automotive and industrial applications [1]. In Gasoline Direct Injection 'GDI' engines, the fuel is supplied to the combustion chamber during the compression stroke in the form of sprays [2], which consist of droplet streams. Droplets in these streams are broken up, heated and evaporated, and these processes

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take place almost simultaneously. They affect the mixture preparation (air + fuel vapour) and the physical ignition delay [3].

Models for heating and evaporation of fuel droplets can be classified based on fuel composition: models based on the assumption that fuel is mono-component and those taking into account the multi-component composition of the fuel. Models taking into account the multi-component composition of fuel are very important and relevant for practical applications and our analysis will be focused upon them. This group of models can be further subdivided into two subgroups: those applicable for a small number of components (Discrete Component Model (DCM)) [4]-[15] and those applicable for large numbers of components (e.g. Continuous Thermodynamics approach [16]-[23] and the Distillation Curve Model [24]). In the first subgroup, the choice of discrete components could be based on either the pseudo-components or the key components approach [16]. The pseudo-components approach is based on replacing the continuous distribution of the mixture with a discrete one. The key components approach is based on replacing the continuous mixture with components with thermodynamics properties similar to those of the continuous mixture [16]. In the second subgroup a number of additional simplifying assumptions are used including the assumption that species mix infinitely quickly inside the droplet or do not mix at all.

In [3,25], it was pointed out that the effects of finite thermal conductivity and recirculation inside the droplets need to be taken into account in modelling droplet heating and evaporation. The simplest approach to doing this can be based on the application of the Effective Thermal Conductivity (ETC) model [28,29]. Also, in [12,13], which focused on the modelling of heating and evaporation of bi-component droplets, it was demonstrated that the effect of finite diffusivity and recirculation of liquid species cannot be ignored. These effects were taken into account based on the Effective Diffusivity (ED) model.

A quasi-discrete model for heating and evaporation of complex mixtures with large numbers of components was suggested in [26]. This model is based on replacing a large number of actual components with a small number of quasi-components to approximate complex mixtures. The version of this model developed in [26] is based on the assumption that fuel consists only of alkanes (C_nH_{2n+2}). These quasi-components are then treated as actual components with averaged values of the carbon number n, taking into account the effect of finite

thermal conductivity and species diffusivities within the liquid droplet. It was assumed that the liquid density, viscosity, heat capacity and thermal conductivity of all quasi-components are the same as those for *n*-dodecane, while the values of latent heat of evaporation and saturated vapour pressure take into account the effect of the number of carbon atoms as suggested in [21]. This model was applied for the analysis of heating and evaporation of Diesel fuel approximated by 21 components. These correspond to a maximum of 20 quasi-components, having average properties between those for neighbouring alkanes with the difference between carbon numbers equal to 1. It was demonstrated that the predictions of the model with 5 quasi-components are very close to the predictions of the model that includes contributions from all 20 quasi-components.

In [27], the original quasi-discrete model was generalised to take into account the dependence of liquid density, viscosity, heat capacity and thermal conductivity on the number of carbon atoms. The new model was applied to the analysis of heating and evaporation of both Diesel (approximated by 21 components or maximum 20 quasi-components) and gasoline (approximated by 14 components or maximum 13 quasi-components) fuels. As in [26], it was demonstrated that in the case of Diesel fuel the results predicted using 5 quasi-components are almost indistinguishable from the results predicted by the model taking into account the contribution of all 20 quasi-components. In the case of gasoline fuel the results predicted using 3 quasi-components were very close to the results predicted by the model taking into account the contribution of 13 quasi-components. This demonstrates the potential usefulness of the quasi-discrete model for the analysis of heating and evaporation of droplets consisting of many components.

A number of authors have attempted to approximate gasoline fuels with various surrogates based on fuel ignition characteristics. In [30] the autoignition characteristics of gasoline/air and ternary surrogate/air mixtures behind reflected shock waves in conditions similar to those found in homogeneous charge compression ignition (HCCI) engine cycles were studied. Two surrogates were considered: Surrogate A (molar fractions: 56% C_7H_{16} + 28% C_8H_{18} + 17% C_7H_8) and Surrogate B (molar fractions: 63% C_7H_{16} + 20% C_8H_{18}+ 17% C_7H_8). The range of experiments covered combustion of fuel in air for lean, stoichiometric, and rich mixtures (Φ = 0.5, 1.0, 2.0), two pressure ranges (15–25 and 45–60 atm), temperatures from 850

to 1280 K, and exhaust gas recirculation (EGR) loadings of 0, 20, and 30%. Strong agreement was seen between ignition delay time measurements for RD387 gasoline and Surrogate B fuels. In our paper, the feasibility of using Surrogates A or B for the analysis of gasoline fuel droplet heating and evaporation will be investigated. We anticipate that our conclusions could be potentially extended to other surrogate approximations of gasoline fuels, based on the ignition characteristics (e.g. [31]).

The main focus of this paper is to perform an analysis of heating and evaporation of gasoline fuel droplets, assuming that this fuel can be approximated by the above-mentioned surrogate fuels, inferred from the study of fuel ignition characteristics, and by the set of quasi-components, inferred from the quasi-discrete model. The models used in our analysis are briefly described in Section 2. The results of the application of these models to the analysis of heating and evaporation of gasoline fuel droplets are presented and discussed in Section 3. The most important results are summarized in Section 4.

2. Model

2.1 Liquid Heat and Mass Transfer

Our analysis is based on the analytical solutions to the one-dimensional heat conduction and species diffusion equations inside spherically-symmetric droplets implemented in the numerical code [25,28,12].

The Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model has been used in our analysis [12,29]. This model takes into account the effect of finite thermal and mass diffusivities alongside the effect of recirculation inside the droplet [12].

The effects of coupling between the droplet and the surrounding gas and the effects of thermal radiation are ignored at this stage.

2.2 Quasi-discrete model

Following [26,27], the molar mass is used to describe the continuous distribution of gasoline fuel which is assumed to consist only of *n*-alkanes C_nH_{2n+2}. The molar mass (kg/kmole) of *n*-alkane components is related to the number of carbon atoms n as:

$$M(n) = 14n + 2. \quad (1)$$

The distribution function was taken as [21]:

$$f_m(n) = C_m(n_0, n_f)\frac{(M(n)-\gamma)^{\alpha-1}}{\beta^{\alpha}\Gamma(\alpha)}\exp\left[-\left(\frac{M(n)-\gamma}{\beta}\right)\right], \quad (2)$$

where $n_0 = 5 \leq n \leq n_f = 18$, subscripts 0 and f stand for initial and final values of n, $\Gamma(\alpha)$ is the Gamma function, $\alpha = 5.7$ and $\beta = 15$ are parameters that determine the shape of the distribution (they are taken to be the same as in [21]), γ is the origin of the distribution function and is set to 0, and C_m is the normalisation constant and is calculated based on Eq. (4) of [27]. f_m is defined for the range of n between n_0 and n_f and is 0 outside this range. The distribution function was chosen to reproduce the distillation curve for gasoline as specified in ASTM D439 [17]. Following [21], it was truncated at *n*-pentane and it was assumed that gasoline fuel consists only of *n*-alkanes with $18 \geq n \geq 5$ for liquid fuels. This distribution function is shown in Fig. 1.

The dependence of the latent heat of evaporation, vapour pressure, liquid density, viscosity, specific heat capacity and thermal conductivity on the number of carbon atoms are taken into account as in [27].

Following [26,27], the continuous distribution (2) is replaced with a discrete one, consisting of N_f quasi-components with carbon numbers:

$$\bar{n}_j = \frac{\int_{n_{j-1}}^{n_j} n f_m(n)\mathrm{d}n}{\int_{n_{j-1}}^{n_j} f_m(n)\mathrm{d}n}. \quad (3)$$

The corresponding molar and mass fractions are found as

$$X_j = \int_{n_{j-1}}^{n_j} f_m(n)\mathrm{d}n, \quad (4)$$

$$Y_j = \frac{M(\bar{n}_j)X_j}{\sum_{j=1}^{j=N_f}[M(\bar{n}_j)X_j]}, \quad (5)$$

where j is an integer in the range $1 \leq j \leq N_f$.

Equations (3-5) are applied to each quasi-component using relevant values of n_j and n_{j-1}.

The diffusion coefficient between quasi-components is assumed to be the same for all quasi-components and it is calculated using Eq. (22) of [26]. The viscosity of liquid gasoline fuel, used in the ETC/ED model, is assumed to be the same as for *n*-octane [36].

$$\mu_{gf} = 0.001 * 10^{(-5.9245+8.8809\times10^{2}\times T+1.2955\times10^{-2}\times T^{-1}-1.3596\times10^{-5}\times T^{2})}. \quad (6)$$

All other thermo-physical properties of the mixture and the vapour diffusion coefficient are calculated as in [12]. The properties of the quasi-components in the quasi-discrete model are the same as discussed in [27]. The thermo-physical properties of n-heptane and iso-octane, two components used in Surrogates A and B, are assumed to be the same as in [33] and [34], respectively. The physical properties of toluene, the third component used in Surrogate A and B, are taken from [35,36]. The vapour pressure for each component was calculated based on the Clausius-Clapeyron equation [12].

3. Results

A plot of $f_m(n)$ versus n for gasoline fuel, using values of parameters (α, β, γ) given in [21,27], is shown in Fig. 1. As can be seen from this figure, the value of n for which $f_m(n)$ is maximal is equal to 5. The average value of n is estimated as $\bar{n}_j = \mathbf{7.05}$, which is reasonably close to $n = 8$ (*n*-octane), a commonly used approximation for gasoline fuel.

We focus on a comparative analysis of the effects of various approximations of gasoline fuel, discussed in Section 2, on fuel droplet heating and evaporation. The following approximations were considered. Firstly we looked at the approximation of gasoline fuel by three quasi-components (molar fractions: 83.0% *n*-$C_{6.26}H_{14.58}$ + 15.6% *n*-$C_{10.24}H_{22.48}$ + 1.4% *n*-$C_{14.42}H_{30.84}$) as suggested in [27] (see Fig. 1 and Table 1). Secondly, we considered the approximations of these quasi-components by two surrogates with *n* rounded up and down to the nearest integers: Surrogate I (mole fractions: 83.0% *n*-C_6H_{14} + 15.6% *n*-$C_{10}H_{22}$ + 1.4% *n*-$C_{14}H_{30}$), Surrogate II (molar fractions: 83.0% *n*-C_7H_{16} + 15.6% *n*-$C_{11}H_{24}$ + 1.4% *n*-$C_{15}H_{32}$) (see Table 1). These surrogates allowed us to investigate the sensitivity of the results to the choice of the values of the number of carbon atoms for each quasi-component ($\bar{n}_1$, $\bar{n}_2$ and $\bar{n}_3$). Also, this rounding up or down of the values of the carbon numbers would allow us to use these approximations of quasi-components in Computational Fluid Dynamics (CFD) codes, which do

not recognise substances with non-integer n. Thirdly, we looked at the approximations of gasoline fuel by gasoline Surrogates A and B considered in [30] (see Table 1). Surrogates of the third group were chosen based of their ignition characteristics. Nobody, to the best of our knowledge, has explored the usefulness of these surrogates in investigation of gasoline fuel droplet heating and evaporation. The results obtained based on the above approximations will be compared with the results based on the approximation of gasoline fuel by 13 quasi-components and the simplistic case of one quasi-component, both based on the distribution function shown in Fig. 1, as discussed in [27].

The plots of droplet surface temperatures T_s and radii R_d versus time for the five surrogates, shown in Table 1, and the approximations of gasoline fuel by 1 (n-$C_{7.05}H_{16.1}$) and 13 quasi-components are presented in Fig. 2. The initial droplet radii and temperatures are assumed equal to 10 μm and 300 K respectively in all cases; the droplet velocities are assumed to be constant and equal to 10 m/s, while gas temperature and pressure are assumed equal to 450 K and 0.3 MPa respectively. The calculations were performed using the ETC/ED model. It can be seen from this figure that the predicted temporal variations of droplet surface temperatures and radii for Surrogates A and B and approximation of gasoline fuel with 1 quasi-component are qualitatively different from the predictions taking into account the contributions of all 13 quasi-components, assumed to be the most accurate approximation of this fuel. It can be seen that Surrogates A and B behave as almost one component and this can be attributed to the closeness of the boiling points of the individual components of these surrogates. At the same time, the predictions for gasoline fuel by 3 quasi-components and Surrogates I and II are reasonably close to the predictions based on consideration of 13 quasi-components. This closeness is particularly visible in the case of Surrogate II.

The choice of 3 quasi-components and Surrogates I and II was made to perform a 'like-with-like' comparison with the model based on Surrogates A and B, based on three components. We appreciate that the approximation of realistic gasoline fuel by three quasi-components used in this paper has a number of limitations. Firstly, this approximation, based on the quasi-discrete model, does not take into account the contribution of other components apart from n-alkanes. Secondly, the approximation of the actual molar fractions of the n-alkane components by distribution (2) could be rather crude. The first limitation is unavoidable due to the current state

of development of the quasi-discrete model. The second limitation could be avoided if a more accurate approximation were available. Whilst these limitations exist we have no other choice but to use the distribution used in [21,27].

The longest evaporation time and highest droplet surface temperature at the end of evaporation is predicted for the 13 quasi-components mixture. This is due to the contribution of heavy alkanes in the mixture. It is further observed that there are 3 heating-up periods for the approximation based on 3 quasi-components and Surrogates I and II. These periods are not observed for other mixtures. This can be attributed to the fact that the approximation based on 3 quasi-components and Surrogates I and II contains hydrocarbons with a wide range of carbon atoms, in contrast to other mixtures. The wide range of carbon atoms leads to significant differences in the thermo-physical properties of the mixture components [26,27].

The limitations of using 1 quasi-component for the analysis of gasoline fuel droplet heating and evaporation were discussed earlier in [27]. As follows from Fig. 2, the replacement of 1 quasi-component with Surrogates A or B does not improve the situation. Hence, although Surrogates A and B can be used for approximation of the autoignition characteristics of gasoline fuel, they are not suitable approximations for the analysis of gasoline fuel droplet heating and evaporation.

Also, one can see from Fig. 2 that the predicted surface temperatures and radii are rather sensitive to the values of the carbon numbers, which is illustrated by the difference in predictions of these parameters by the approximations of gasoline fuel by 3 quasi-components and Surrogates I and II. This could potentially open the way to improving the predictions of the quasi-discrete models by replacing the approximation based on 3 quasi-components with non-integer n with Surrogate II. However, further investigations would be required before we are able to issue this recommendation. This would include the analysis of possible contributions of other hydrocarbons (apart from *n*-alkanes) in rigorous approximations of gasoline fuels, and the analysis of fuel droplet heating and evaporation for a wide range of parameters. Before this is done, our analysis will focus primarily on the approximation based of 3 quasi-components, as in [27].

The plots of liquid molar fractions at the surface of the droplets $X_{ls,j=1,2,3}$ versus time for all 3 quasi-components are shown in Fig. 3. The values of $X_{ls,1}$ (lighter component) and $X_{ls,3}$ (heavier component) monotonically decrease and increase with time respectively. The behaviour of $X_{ls,2}$ is different where it initially increases with time and then starts to decrease with time after the lighter component has fully evaporated. This behaviour is similar to that shown in Fig 11 of [27] for 4 quasi-components. It is consistent with our observation that the model based on 3 quasi-components predicts longer evaporation times and larger droplet surface temperatures at the final stages of droplet evaporation, compared with the model using 1 quasi-component.

4. Conclusions

Effects of fuel approximations and initial values of various parameters on heating and evaporation of gasoline droplets are investigated. The following approximations are considered: 3 quasi-components introduced in the quasi-discrete model and their approximations: Surrogate I (molar fractions: 83% *n*-C_6H_{14} + 15.6% *n*-$C_{10}H_{22}$ + 1.4% *n*-$C_{14}H_{30}$) and Surrogate II (molar fractions: 83% *n*-C_6H_{14} + 15.6% *n*-$C_{10}H_{22}$ + 1.4% *n*-$C_{14}H_{30}$)), surrogate approximations of gasoline fuel based on its ignition characteristics: Surrogate A (molar fractions: 56% *n*-C_7H_{16} + 28% *iso*-C_8H_{18} + 17% C_7H_8) and Surrogate B (molar fractions: 63% *n*-C_7H_{16} + 20% *iso*-C_8H_{18}+ 17% C_7H_8). The results are compared with the predictions of the model based on the approximation of gasoline fuel by 13 and 1 quasi-components. It has been shown that the predictions of the quasi-discrete model based on the approximation of gasoline fuel with three quasi-components, especially Surrogate II, are much more accurate than those based on other surrogate approximations compared with the predictions of the quasi-discrete model based on 13 quasi-components. This demonstrates the limitation of using fuel surrogates, proposed based on fuel ignition characteristics, for the analysis of liquid fuel droplet heating and evaporation.

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Figure captions

Fig. 1 A plot of $f_m(n)$ versus n for gasoline fuel, as predicted by Eq. (19), showing the 3 quasi-components.

Fig. 2 Plots of droplet surface temperatures T_s and radii R_d versus time, predicted for 1, 3 and 13 quasi-components used in the quasi-discrete model, the approximations of the 3 quasi-components with Surrogates I and II (see Table 1) and Surrogates A and B (see Table 1). The initial droplet radii and temperatures are taken to be equal to 10 μm and 300 K respectively, the droplet velocities equal to 10 m/s, and the gas temperature and pressure, 450 K and 0.3 MPa respectively. The calculations were performed using the ETC/ED model.

Fig. 3 Plots of molar fraction X_{ls} at the surface of the droplet for 3 quasi-components versus time, predicted for the same input parameters as in Fig. 2.

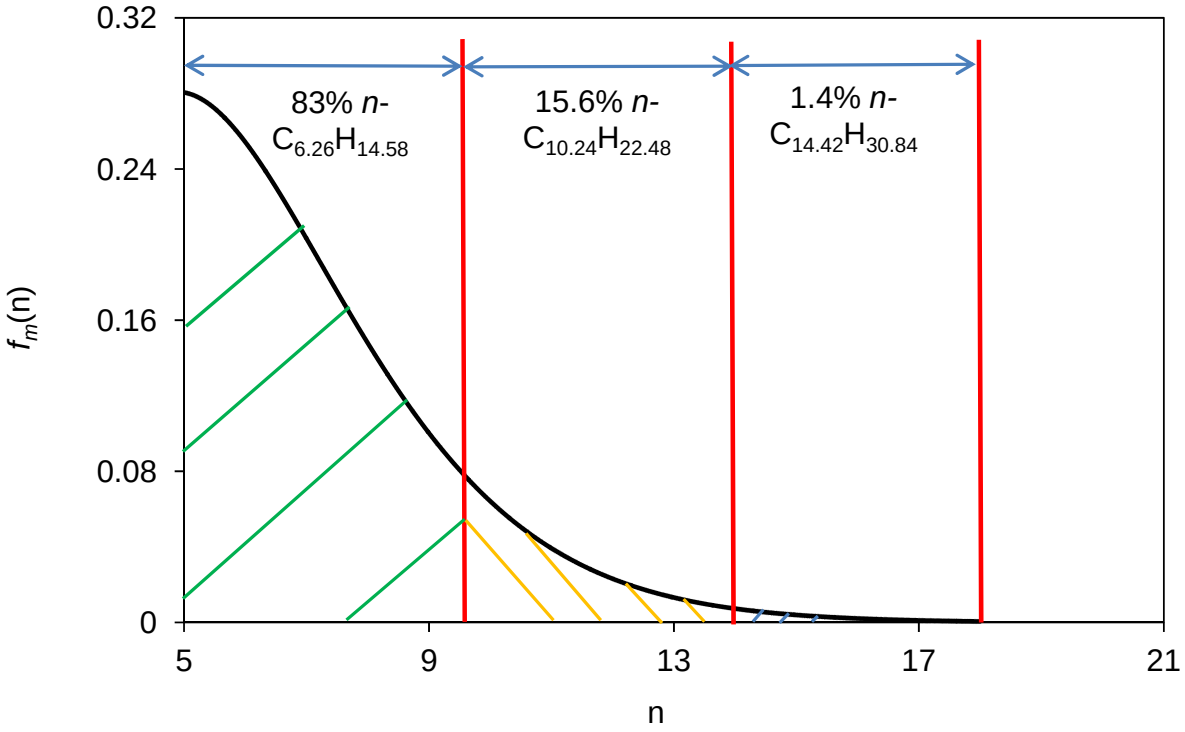
0.32
0.24
0.16
0.08
0
f_m(n)
5
9
13
17
21
n
83% *n*-
$C_{6.26}H_{14.58}$
15.6% *n*-
$C_{10.24}H_{22.48}$
1.4% *n*-
$C_{14.42}H_{30.84}$

Fig. 1

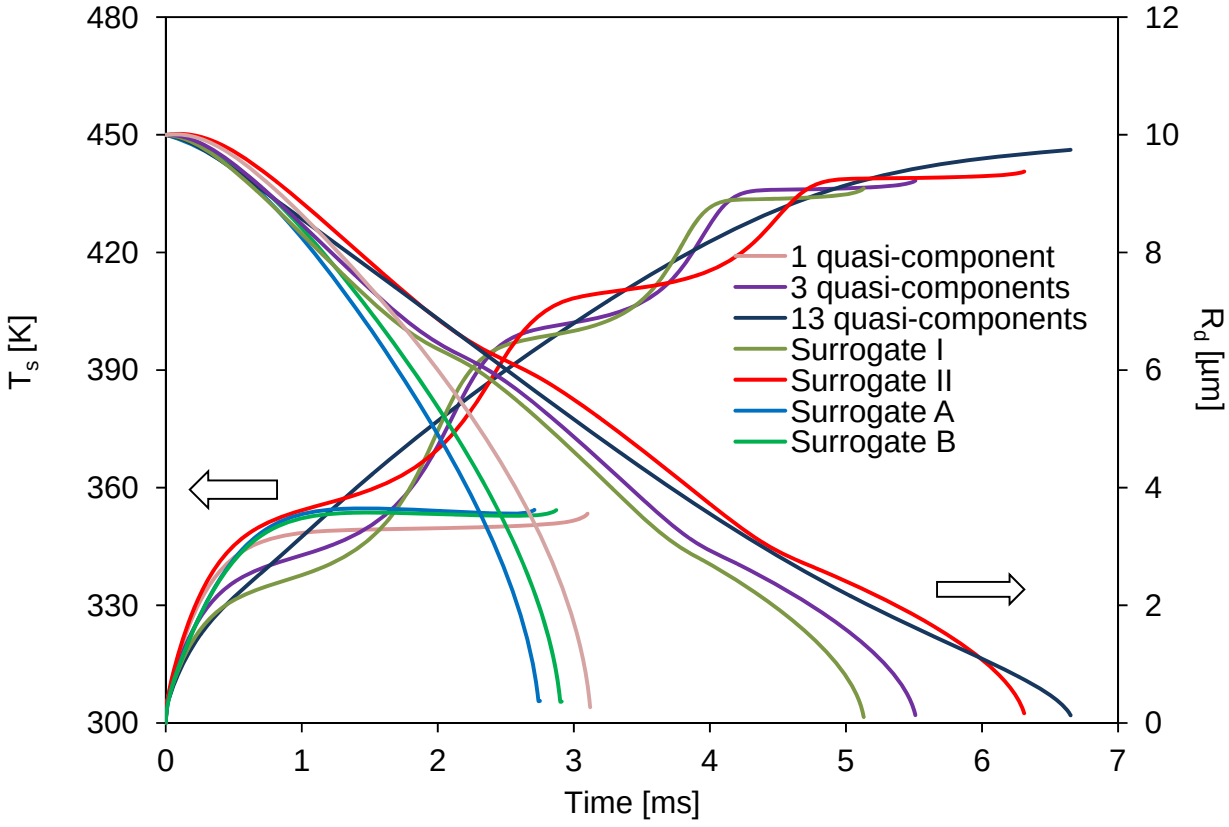
480
450
420
390
360
330
300
12
10
8
6
4
2
0
0
1
2
3
4
5
6
7
Time [ms]
T_s [K]
R_d [μm]
1 quasi-component
3 quasi-components
13 quasi-components
Surrogate I
Surrogate II
Surrogate A
Surrogate B

Fig. 2

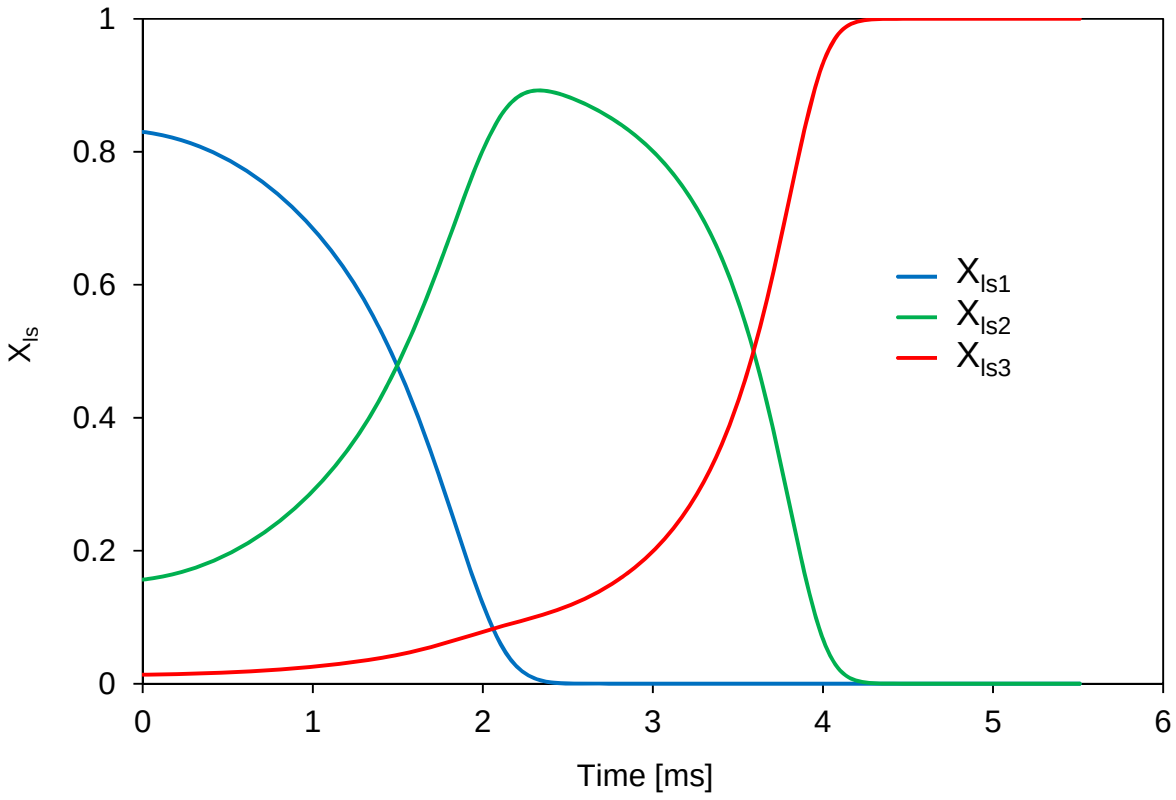

Fig. 3

Tables

Approximation	Ref.	Composition (molar fractions)
1 quasi-component	[27]	*n*-$C_{7.05}H_{16.1}$
3 quasi-components	[27]	83% *n*-$C_{6.26}H_{14.58}$ + 15.6% *n*-$C_{10.24}H_{22.48}$ + 1.4% *n*-$C_{14.42}H_{30.84}$
Surrogate I	new	83% *n*-C_6H_{14} + 15.6% *n*-$C_{10}H_{22}$ + 1.4% *n*-$C_{14}H_{30}$
Surrogate II		83% *n*-C_7H_{16} + 15.6% *n*-$C_{11}H_{24}$ + 1.4% *n*-$C_{15}H_{32}$
Surrogate A	[30]	56% *n*-C_7H_{16} + 28% *iso*-C_8H_{18} + 17% C_7H_8
Surrogate B		63% *n*-C_7H_{16} + 20% *iso*-C_8H_{18} +17% C_7H_8

Table 1. Molar fractions of components in various gasoline fuel approximations and surrogates.