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New approaches to the modelling of multi-component fuel droplet heating and evaporation

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Abstract. The previously suggested quasi-discrete model for heating and evaporation of complex multi-component hydrocarbon fuel droplets is described. The dependence of density, viscosity, heat capacity and thermal conductivity of liquid components on carbon numbers n and temperatures is taken into account. The effects of temperature gradient and quasi-component diffusion inside droplets are taken into account. The analysis is based on the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model. This model is applied to the analysis of Diesel and gasoline fuel droplet heating and evaporation. The components with relatively close n are replaced by quasi-components with properties calculated as average properties of the *a priori* defined groups of actual components. Thus the analysis of the heating and evaporation of droplets consisting of many components is replaced with the analysis of the heating and evaporation of droplets consisting of relatively few quasi-components. It is demonstrated that for Diesel and gasoline fuel droplets the predictions of the model based on five quasi-components are almost indistinguishable from the predictions of the model based on twenty quasi-components for Diesel fuel droplets and are very close to the predictions of the model based on thirteen quasi-components for gasoline fuel droplets. It is recommended that in the cases of both Diesel and gasoline spray combustion modelling, the analysis of droplet heating and evaporation is based on as little as five quasi-components.

1. Introduction

In a number of our earlier papers it was demonstrated that the choice of the model for droplet heating and evaporation leads to a noticeable effect on the predicted autoignition delay in Diesel fuel sprays [1, 2]. It was pointed out that a widely used model for droplet heating and evaporation, based on the assumption that the liquid thermal conductivity is infinitely large, leads to considerable overestimation of the autoignition delay, especially for high gas temperatures. It was recommended that the effect of the finite value of this conductivity be taken into account in spray autoignition modelling using the Effective Thermal Conductivity (ETC) model [3].

One of the main limitations of the analysis presented in [1, 2] is that it was based on the assumption that Diesel fuel can be approximated as a mono-component fuel. This assumption



is obviously too crude for realistic Diesel fuels which consist of hundreds of various components. The models suggested in the literature to deal with such complex fuels are based on the probabilistic analysis of a large number of components (e.g. Continuous Thermodynamics approach [4]-[11], the Distillation Curve Model [12], the combination of the Continuous Thermodynamics approach and the Discrete Component Model [13], and the Quadrature Method of Moments [14, 15]). All these models, however, are based on a number of additional simplifying assumptions, including the assumption that species inside droplets mix infinitely quickly or do not mix at all. As follows from our analysis of heating and evaporation of bi-component droplets [16, 17], this assumption can lead to large errors.

A new approach to the modelling of heating and evaporation of multi-component droplets, suitable for the case when a large number of components is present in the droplets, is suggested in [18, 19]. This approach is based on the introduction of quasi-components, which are treated as hypothetical components, but the number of these quasi-components is much smaller than the number of actual components. In contrast to the previously suggested models, designed for large numbers of components, the new model takes into account the diffusion of liquid species and thermal diffusion. This model was called the ‘quasi-discrete model’.

Despite a number of limitations, we believe that it is the most advanced approach when compared with others suggested for the modelling of heating and evaporation in complex hydrocarbon sprays, including Diesel and gasoline fuel sprays. The modelling of heating and evaporation of these sprays is integral to the modelling of their autoignition.

The aim of this paper is to present a brief summary of the essence of this model and show some new results.

2. Quasi-discrete model

As in the case of the Continuous Thermodynamics approach, the quasi-discrete model is based on the introduction of the distribution function $f_m(I)$ such that:

$$\int_{I_1}^{I_2} f_m(I) dI = 1, \quad (1)$$

where I is the property of the component, f_m characterises the relative contribution of the components having this property in the vicinity of I , I_1 and I_2 are limiting values of this property.

Although molar mass M is almost universally used to describe the property I , this choice is certainly far from being a unique one. Remembering that most practically important hydrocarbon fuels consist mainly of molecules of the type C_nH_{2n+2} (alkanes), where $n \geq 5$ for liquid fuels, it is more practical to write the distribution function f_m as a function of the carbon number n rather than M [9]. Note that

$$M = 14n + 2, \quad (2)$$

where M is measured in kg/kmole.

As in [18] we assume that $f_m(n)$ can be approximated as:

$$f_m(n) = C_m(n_0, n_f) \frac{(M(n) - \gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp \left[- \left(\frac{M(n) - \gamma}{\beta} \right) \right], \quad (3)$$

where $n_0 \leq n \leq n_f$, subscripts $_0$ and $_f$ stand for initial and final, $\Gamma(\alpha)$ is the Gamma function, α and β are parameters that determine the shape of the distribution, γ determines the original shift,

$$C_m(n_0, n_f) = \left\{ \int_{n_0}^{n_f} \frac{(M(n) - \gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp \left[- \left(\frac{M(n) - \gamma}{\beta} \right) \right] dn \right\}^{-1}. \quad (4)$$

This choice of C_m assures that $\int_{n_0}^{n_f} f_m(n)dn = 1$.

As in [18] we use the following approximation for the dependence of the saturation vapour pressure (in MPa) on n :

$$p^{\text{sat}}(n) = \exp\left(A(n) - \frac{B(n)}{T - C(n)}\right), \quad (5)$$

where T is in K,

$$A(n) = 6.318 n^{0.05091}, \quad B(n) = 1178 n^{0.4652}, \quad C(n) = 9.467 n^{0.9143}.$$

From the Clausius-Clapeyron equation it follows that [9]

$$L = -\frac{R_u}{M(n)} \frac{d \ln p^{\text{sat}}(n)}{d(1/T)}, \quad (6)$$

where R_u is the universal gas constant. Remembering (5), Formula (6) can be rewritten as:

$$L = \frac{R_u B(n) T^2}{M(n) (T - C(n))^2}. \quad (7)$$

Following [18], this formula will be used in our analysis.

In [18] the dependence of liquid density, viscosity, specific heat capacity and thermal conductivity on n was ignored. In our analysis this dependence is taken into account, following [19], based on published data for liquid density [20], viscosity [21], specific heat capacity [22] and thermal conductivity [23] (see Figs. A1-A4 of [19]).

As follows from (5), (7) and the results for liquid density, viscosity, specific heat capacity and thermal conductivity, the transport and thermodynamic properties of the fuel components are relatively weak functions of n . In this case, following [18, 19], it would be sensible to assume that the properties of hydrocarbons in a certain narrow range of n are close, and replace the continuous distribution (3) with a discrete one, consisting of N_f quasi-components with carbon numbers

$$\bar{n}_j = \frac{\int_{n_{j-1}}^{n_j} n f_m(n) dn}{\int_{n_{j-1}}^{n_j} f_m(n) dn}, \quad (8)$$

the corresponding molar fractions

$$X_j = \int_{n_{j-1}}^{n_j} f_m(n) dn, \quad (9)$$

and mass fractions

$$Y_j = \frac{M(\bar{n}_j) X_j}{\sum_{j=1}^{N_f} [M(\bar{n}_j) X_j]}, \quad (10)$$

where j is an integer in the range $1 \leq j \leq N_f$. We assume that all $n_j - n_{j-1}$ are equal, i.e. all quasi-components have the same range of values of n . For the case when $N_f = 1$ this approach reduces the analysis of multi-component droplets to mono-component ones.

These new quasi-components are not the actual physical hydrocarbon components (\bar{n}_j are not integers in the general case). Hence we called this model a quasi-discrete model. These quasi-components are treated as actual components in the conventional Discrete Component Model, including taking into account diffusion of liquid species in droplets. This model is expected to be particularly useful when N_f is much less than the number of actual species in the hydrocarbon mixture.

Partial pressures of individual quasi-components can be estimated as (Raoult's law is assumed to be valid):

$$p_v(\bar{n}_j) = X_{lsi}(\bar{n}_j)p^{\text{sat}}(\bar{n}_j), \quad (11)$$

where X_{lsi} is the molar fraction of liquid quasi-components at the surface of the droplet, $p^{\text{sat}}(\bar{n}_j)$ is determined by Eq. (5).

Having replaced n with \bar{n}_j we obtain the required values of p^{sat} , L , liquid density, viscosity, specific heat capacity and thermal conductivity for all quasi-components.

Note that, strictly speaking, the viscosity and thermal conductivity of the mixture are not equal to those for \bar{n}_j (see [24] for details). The difference between them, however, is expected to be relatively small and will be ignored in our analysis.

3. The diffusion of quasi-components

Equations for mass fractions of quasi-components $Y_j \equiv Y_j(t, R)$ inside droplets are used in the following form:

$$\frac{\partial Y_j}{\partial t} = D_l \left(\frac{\partial^2 Y_j}{\partial R^2} + \frac{2}{R} \frac{\partial Y_j}{\partial R} \right), \quad (12)$$

where $j > 1$, D_l is the liquid mass diffusivity. Eq. (12) is solved with the following boundary condition [16, 17]:

$$\alpha(\epsilon_j - Y_{js}) = -D_l \left. \frac{\partial Y_j}{\partial R} \right|_{R=R_d-0}, \quad (13)$$

and the initial condition $Y_j(t=0) = Y_{j0}(R)$, where $Y_{js} = Y_{js}(t)$ are liquid components' mass fractions at the droplet's surface,

$$\alpha = \frac{|\dot{m}_d|}{4\pi\rho_l R_d^2}, \quad (14)$$

R_d is the droplet radius, \dot{m}_d is the rate of mass loss by droplets, ρ_l is the total liquid density.

Assuming that species concentrations in the ambient gas are equal to zero ($Y_{v\infty} = 0$), the values of ϵ_j can be found from the following relation [16]:

$$\epsilon_j = \frac{Y_{vjs}}{\sum_j Y_{vjs}}, \quad (15)$$

where the subscript v indicates the vapour phase. We assume that ϵ_j are still defined by Eq. (15) even in the case when these concentrations are not equal to zero, which is expected in the case of a coupled solution. In contrast to a widely used approach, based on the numerical solution to Eq. (12), our analysis is based on its analytical solution [16, 17]:

$$Y_{li} = \epsilon_i + \frac{1}{R} \left\{ \left[\exp \left[D_l \left(\frac{\lambda_0}{R_d} \right)^2 t \right] [q_{i0} - Q_0 \epsilon_i] \sinh \left(\lambda_0 \frac{R}{R_d} \right) + \sum_{n=1}^{\infty} \left[\exp \left[-D_l \left(\frac{\lambda_n}{R_d} \right)^2 t \right] [q_{in} - Q_n \epsilon_i] \sin \left(\lambda_n \frac{R}{R_d} \right) \right] \right\}, \quad (16)$$

where λ_0 and λ_n ($n \geq 1$) are solutions to equations

$$\tanh \lambda = -\frac{\lambda}{h_0} \quad \text{and} \quad \tan \lambda = -\frac{\lambda}{h_0}.$$

respectively, $h_0 = -\left(1 + \frac{\alpha R_d}{D_l}\right)$,

$$Q_n = \begin{cases} -\frac{1}{\|v_0\|^2} \left(\frac{R_d}{\lambda_0}\right)^2 (1 + h_0) \sinh \lambda_0 & \text{when } n = 0 \\ \frac{1}{\|v_n\|^2} \left(\frac{R_d}{\lambda_n}\right)^2 (1 + h_0) \sin \lambda_n & \text{when } n \geq 1 \end{cases} \quad (17)$$

$$q_{in} = \frac{1}{\|v_n\|^2} \int_0^{R_d} R Y_{li0}(R) v_n(R) dR, \quad n \geq 0, \quad (18)$$

$$v_0(R) = \sinh\left(\lambda_0 \frac{R}{R_d}\right), \quad v_n(R) = \sin\left(\lambda_n \frac{R}{R_d}\right), \quad n \geq 1.$$

The average mass fraction of species in a moving droplet can still be correctly predicted by Equation (12), with appropriate boundary conditions, if the liquid diffusivity D_l is replaced with the so-called effective diffusivity D_{eff}

$$D_{\text{eff}} = \chi_Y D_l, \quad (19)$$

where the coefficient χ_Y varies from 1 to 2.72 and can be approximated as:

$$\chi_Y = 1.86 + 0.86 \tanh[2.225 \log_{10}(\text{Re}_l \text{Sc}_l / 30)], \quad (20)$$

Re_l is the Reynolds number, based on liquid transport properties and the maximum surface velocity inside droplets, Sc_l is the liquid Schmidt number.

The analytical solution (16) is incorporated into the numerical scheme when the effect of droplet evaporation is taken into account. Recirculation inside droplets is taken into account based on the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model [16, 17]. The solution described in [16, 17] has been generalised in [25] to take into account the effect of the moving droplet boundary due to the evaporation process.

4. Application to Diesel and gasoline fuel droplets

Following [9] we assume the following values of parameters for the distribution function (3) for Diesel and gasoline fuels.

Fuel	α	β (kg/kmole)	γ (kg/kmole)	n_0	n_f
Diesel	18.5	10	0	5	25
Gasoline	5.7	15	0	5	18

Table 1

As in [18, 19], we assumed that the initial Diesel fuel droplet temperature is equal to 300 K, and is homogeneous throughout its volume. Gas temperature and pressure are assumed to be equal to 880 K and 3 MPa respectively. The initial composition of droplets is described by distribution function (3) with the values of parameters given in Table 1.

Plots of droplet surface temperature T_s and radius R_d versus time for the initial radius equal to 10 μm and velocity 1 m/s are shown in Fig. 1. The droplet velocity is assumed to be constant during the whole process. The calculations were performed for the case of $N_f = 1$ (one quasi-component droplet, $\bar{n} = 12.56$), $N_f = 5$ (five quasi-component droplet) and $N_f = 20$ (twenty quasi-component droplet), using the ETC/ED model. The latter case is expected to reproduce adequately the properties of actual Diesel fuels [9].

As one can see from this figure, the droplet radii R_d and surface temperature T_s , predicted by the ETC/ED model, using one and twenty quasi-components are noticeably different,

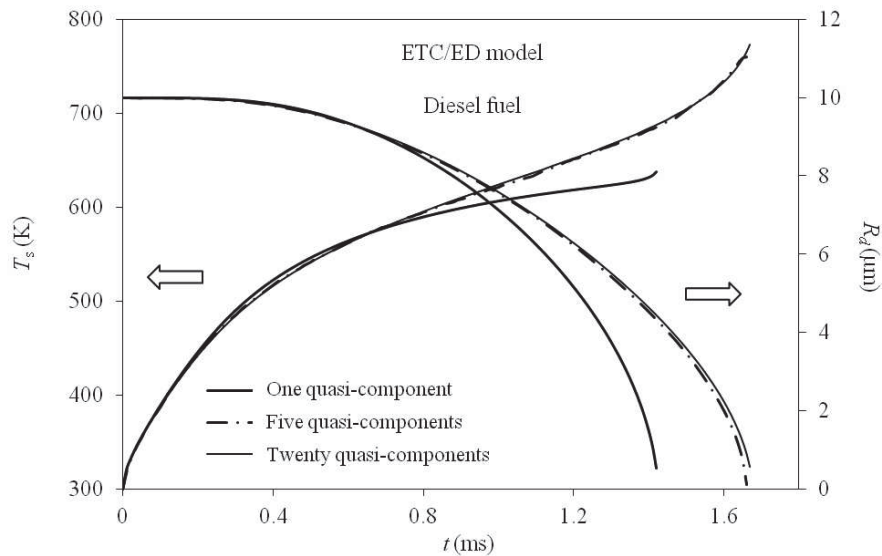


Figure 1. Plots of T_s and R_d , predicted by the ETC/ED model, versus time for 1, 5 and 20 quasi-components. The initial droplet radius and temperature are assumed to be equal to $10 \mu\text{m}$ and 300 K respectively; the droplet velocity is assumed to be equal to 1 m/s and its changes during the heating and evaporation process are ignored; gas temperature is assumed equal to 880 K .

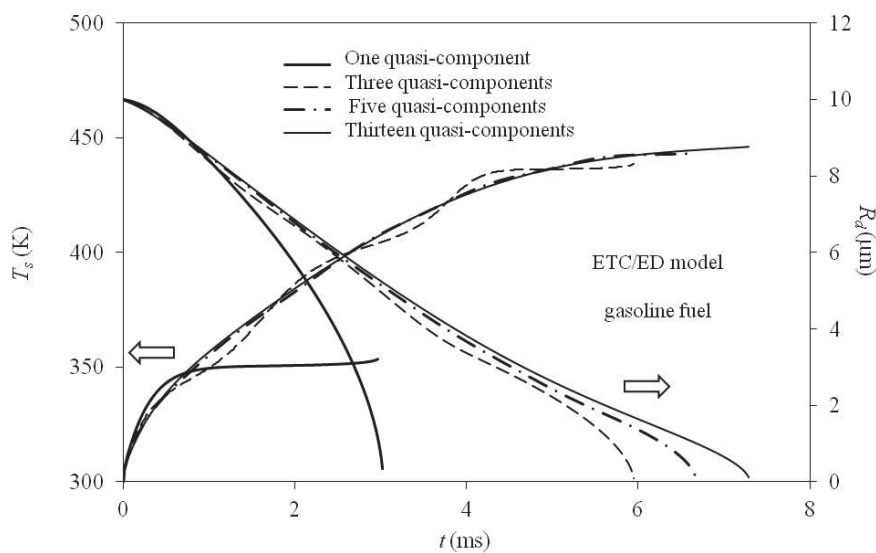


Figure 2. The same as Fig. 1 but for gasoline fuel droplets with velocity equal to 10 m/s , gas temperature equal to 450 K and pressure equal to 0.3 MPa .

especially at the final stages of droplet heating and evaporation. The model, using twenty quasi-components predicts higher surface temperatures and longer evaporation time compared with the model using one quasi-component. This can be related to the fact that at the final stages of droplet evaporation the species with large n become the dominant. These species evaporate more slowly than the species with lower n and have higher wet bulb temperatures. At

the same time, the predictions of the model using just five quasi-components are almost identical with the predictions of the model using twenty quasi-components, in agreement with the earlier results reported in [18].

Plots similar to those shown in Fig. 1, but for gasoline fuel droplets in realistic conditions for gasoline engines, are presented in Fig. 2. Following [26], we assume that gas temperature is equal to 450 K, gas pressure is equal to 0.3 MPa and droplet velocity is equal to 10 m/s. As in the case shown in Fig. 1, we assumed that the initial droplet temperature is equal to 300 K, and is homogeneous throughout its volume, while the droplet initial radius is equal to 10 μm .

The calculations were performed for the case of $N_f = 1$, $N_f = 3$, $N_f = 5$ and $N_f = 13$, using the ETC/ED model. The latter case is expected to reproduce adequately the properties of actual gasoline fuels [9].

Comparing Figs. 1 and 2, one can see that in the latter case the difference between the predicted temperatures and droplet radii for one and thirteen quasi-components is much more visible than in the former. This can be attributed to much slower evaporation for the case shown in Fig. 2, compared with the case shown in Fig. 1. At the same time, the predictions of the model using just three and especially five quasi-components are reasonably close to the predictions of the model using thirteen quasi-components. The general trends of the curves shown in Fig. 2 are similar to the ones shown in Fig. 1. In the case when thirteen quasi-components are considered, at the end of the evaporation process, mainly the heavier components in the droplets remain. These can reach higher temperatures and evaporate more slowly compared with the light and middle-range components.

Note that the analysis described above is based on the hydrodynamic model for droplet evaporation. The kinetic and molecular dynamic effects will be taken into account during further developments of this model. Some of the most recent results in this direction are described in [27, 28].

5. Conclusions

The previously suggested quasi-discrete model for heating and evaporation of complex multi-component hydrocarbon fuel droplets is described. The dependence of density, viscosity, heat capacity and thermal conductivity of liquid components on carbon numbers and temperatures is taken into account. This model is applied to the modelling of Diesel and gasoline fuel droplet heating and evaporation.

The model is based upon the assumption that properties of the components vary relatively slowly from one component to another and depend on a single parameter: the number of carbon atoms in the components (carbon number: n). The components with relatively close n are replaced with quasi-components with properties calculated as average properties of the *a priori* defined groups of actual components. Thus the analysis of the heating and evaporation of droplets consisting of many components is replaced with the analysis of the heating and evaporation of droplets consisting of relatively few quasi-components. The effects of temperature gradient and quasi-component diffusion inside droplets are taken into account. The analysis is based on the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model.

It is demonstrated that for Diesel fuel droplets the predictions of the model based on five quasi-components are almost indistinguishable from the predictions of the model based on twenty quasi-components (maximal number of quasi-components). These are noticeably different from the predictions of the model, based on one quasi-component, widely used in spray combustion modelling. A similar conclusion was drawn for gasoline fuel droplets with the maximal number of quasi-components equal to thirteen. It is recommended that in the cases of both Diesel and gasoline spray combustion modelling, the analysis of droplet heating and evaporation is based on five quasi-components.

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