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Modelling of biodiesel fuel droplet heating and evaporation

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HIGHLIGHTS

- Discrete Components Model taking into account liquid species diffusion.
- The dependence of the properties of components of biodiesel fuels on temperature.
- The modelling of heating and evaporation of biodiesel fuel droplets.

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ABSTRACT

Biodiesel fuel droplet heating and evaporation is investigated using the previously developed models, taking into account temperature gradient, recirculation, and species diffusion within droplets. The analysis is focused on four types of biodiesel fuels: Palm Methyl Ester, Hemp Methyl Esters, Rapeseed oil Methyl Ester, and Soybean oil Methyl Ester. These fuels contain up to 15 various methyl esters and possibly small amounts of unspecified additives, which are treated as methyl esters with some average characteristics. Calculations are performed using two approaches: (1) taking into account the contribution of all components of biodiesel fuels (up to 16); and (2) assuming that these fuels can be treated as a one component fuel with averaged transport and thermodynamic coefficients. It is pointed out that for all types of biodiesel fuel the predictions of the multi-component and single component models are rather close (the droplet evaporation times predicted by these models differ by less than about 5.5%). This difference is much smaller than observed in the case of Diesel and gasoline fuel droplets, and is related to the fact that in the case of Diesel and gasoline fuel droplets the contribution of components in a wide range of molar masses and enthalpies of evaporation needs to be taken into account, while in the case of biodiesel fuels the main contribution comes from the components in a narrow range of molar masses, boiling temperatures and enthalpies of evaporation. As in the case of Diesel and gasoline fuel droplets, the multi-component model predicts higher droplet surface temperature and longer evaporation times than the single component model.

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1. Introduction

Depletion of fossil fuels and the need to reduce carbon dioxide emissions, contributing to climate changes, have stimulated the development of alternative fuels for internal combustion engines. As an alternative to Diesel fuel biodiesel fuels have been developed [1]. The term 'biodiesel' typically refers to "a fuel comprised of mono-alkyl esters of long-chain fatty acids derived from vegetable oils or animal fats" [2]. Sometimes it is used to refer to as "fatty acid methyl or ethyl esters made from vegetable oils or animal fats, whose properties are good enough to be used in diesel engines" [1]. Biodiesel is produced from vegetable oil or animal fat through the process known as transesterification [3]. Most studies of biodiesel fuels have been focused on rapeseed, soybean and palm oil biodiesels [5]. The dominant oils for production of these fuels are rapeseed oil in Europe, soybean oil in the USA, and palm oil in Asia [2]. The term 'second-generation biodiesel' refers to biodiesel derived from inedible oil or algae [4].

Our paper is focused on the modelling of biodiesel fuel droplet heating and evaporation, which is an important stage of the process leading from the injection of biodiesel fuel into a combustion chamber to its ultimate combustion, producing the driving force for internal combustion engines. A number of models of biodiesel fuel heating and evaporation of various complexities have been suggested (e.g. [6,7]). These models either ignored temperature gradients and species diffusion inside droplets or took them into account based on the numerical solutions of the underlying partial

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differential equations (e.g. [7]). The importance of taking into account these effects has been discussed in a number of our previous papers, including [8,9]. In contrast to almost all previous investigations of these processes, the authors of [8,9] based their analysis not on the numerical solutions of the equations for heat transfer and species diffusion in droplets, but on their analytical solutions, which were incorporated into a numerical algorithm.

This approach has been applied to the modelling of droplet heating and evaporation for binary mixtures and for simplified models of Diesel and gasoline fuels. The focus of our paper is on the application of this approach to modelling the heating and evaporation of droplets of various realistic biodiesel fuels in conditions typical for Diesel engines.

The model used in our analysis is briefly described in Section 2. The implementation of this model into a numerical algorithm is summarised in Section 3. Input parameters used in our analysis and the results of calculations are presented and discussed in Sections 4 and 5. The main results of the paper are summarised in Section 6.

2. The model

The main ideas of the model used in our analysis are rather similar to those behind the one described in [8]. This model takes into account the effects of multi-component droplet heating by convection, its evaporation, the finite thermal conductivity, recirculation, and species diffusion in the liquid phase. Only the effects of ambient gas on droplets are taken into account, the effects of coupling between gas and droplets are ignored (see [9] for a possible approach to describe this coupling).

2.1. Droplet heating

The process of heating of mono- and multi-component droplets is described by the following transient heat conduction equation for the temperature $T \equiv T(t,R)$ in the liquid phase [10,11]:

$$\frac{\partial T}{\partial t} = \kappa\left(\frac{\partial^2 T}{\partial R^2} + \frac{2}{R}\frac{\partial T}{\partial R}\right), \tag{1}$$

where $\kappa = k_{\text{eff}}/(c_l\rho_l)$ is the effective thermal diffusivity, k_{eff}, c_l, and ρ_l are the effective thermal conductivity, specific heat capacity, and density respectively, R is the distance from the centre of the droplet (assumed to be spherical), t is time. k_{eff} is linked with the liquid thermal conductivity k_l via the following equation:

$$k_{\text{eff}} = \chi k_l, \tag{2}$$

where the coefficient χ varies from 1 (at droplet Peclet number $\text{Pe}_{d(l)} = \text{Re}_{d(l)}\text{Pr}_l < 10$) to 2.72 (at $\text{Pe}_{d(l)} > 500$) and can be approximated as [12]:

$$\chi = 1.86 + 0.86\tanh\left[2.225\log_{10}(\text{Pe}_{d(l)}/30)\right]. \tag{3}$$

Liquid fuel transport properties and the liquid velocity just below the droplet surface (see [12] for details) were used for calculating $\text{Pe}_{d(l)}$. The model based on Eqs. (2) and (3) is known as the Effective Thermal Conductivity (ETC) model. When writing Eq. (1) we assumed that droplet sphericity is not affected by its motion [12].

Eq. (1) is to be solved for $t > 0$ and $0 \leqslant R < R_d$, where R_d is the droplet radius, with the following boundary condition, assuming that the effects of evaporation can be ignored:

$$h(T_g - T_s) = k_{\text{eff}}\left.\frac{\partial T}{\partial R}\right|_{R=R_d-0}, \tag{4}$$

and the initial condition $T(t = 0) = T_{d0}(R)$, where $T_s = T_s(t)$ is the droplet's surface temperature, $T_g = T_g(t)$ is the ambient gas temperature, h is the convection heat transfer coefficient, linked with the Nusselt number Nu via the following equation $\text{Nu} = 2R_d h/k_g$, k_g is the gas thermal conductivity. We assume that fuel vapour is dilute and k_g is equal to the thermal conductivity of air. Remembering the physical background to the problem, we are interested only in a solution which is continuously differentiable twice in the whole domain. This implies that T should be bounded for $0 \leqslant R < R_d$.

Assuming that h = const, the solution to Eq. (1), subject to the above boundary and initial conditions, can be presented as [13]:

$$T(R,t) = \frac{1}{R}\sum_{n=1}^{\infty}\left\{q_n \exp\left[-\kappa_R\lambda_n^2 t\right] - \frac{R_d^2\sin\lambda_n}{\|v_n\|^2\lambda_n^2}\mu_0(0)\exp\left[-\kappa_R\lambda_n^2 t\right]\frac{R_d^2\sin\lambda_n}{\|v_n\|^2\lambda_n^2}\int_0^t\frac{d\mu_0(\tau)}{d\tau}\exp\left[-\kappa_R\lambda_n^2(t-\tau)\right]d\tau\right\}\sin\left[\lambda_n\left(\frac{R}{R_d}\right)\right] + T_g(t), \tag{5}$$

where λ_n are solutions to the equation:

$$\lambda\cos\lambda + h_0\sin\lambda = 0, \tag{6}$$

$$\|v_n\|^2 = \frac{R_d}{2}\left(1 - \frac{\sin 2\lambda_n}{2\lambda_n}\right) = \frac{R_d}{2}\left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right),$$

$$q_n = \frac{1}{\|v_n\|^2}\int_0^{R_d}\widetilde{T}_0(R)\sin\left[\lambda_n\left(\frac{R}{R_d}\right)\right]dR, \kappa_R = \frac{k_{\text{eff}}}{c_l\rho_l R_d^2}, \mu_0(t) = \frac{hT_g(t)R_d}{k_{\text{eff}}},$$

$h_0 = (h\,R_d/k_{\text{eff}}) - 1$, $\widetilde{T}_0(R) = RT_{d0}(R)$. The solution to Eq. (6) gives a set of positive eigenvalues λ_n numbered in ascending order ($n = 1, 2, \ldots$). The trivial solution $\lambda = 0$ is not considered.

Solution (5) is valid for $h_0 > -1$, which is satisfied, remembering the physical background of the problem ($h > 0$). The condition h = const is valid for sufficiently small time steps. To take into account the effect of droplet evaporation in analytical solution (5), gas temperature should be replaced by the so-called effective temperature defined as:

$$T_{\text{eff}} = T_g + \frac{\rho_l L\dot{R}_d}{h}, \tag{7}$$

where L is the latent heat of evaporation, the value of $\dot{R}_d$ can be taken from the previous time step and estimated based on Eq. (25). R_d is assumed constant in the analytical solutions, but is updated at the end of the time step Δt: $R_{d(\text{new})} = R_{d(\text{old})} + \dot{R}_d\Delta t$, where the value of $\dot{R}_d$ is controlled by the droplet evaporation model (see Eq. (25) in Section 2.3).

In the limit $k_{\text{eff}} \to \infty$ the prediction of Expression (5) is identical to the one which follows from the model based on the assumption that $k_{\text{eff}} = \infty$ [14] (Infinite Thermal Conductivity (ITC) model). The value of Nu for an isolated moving droplet is estimated based on the following equation [12]:

$$\text{Nu}_{\text{iso}} = 2\frac{\ln(1+B_T)}{B_T}\left(1 + \frac{(1+\text{Re}_d\text{Pr}_d)^{1/3}\max\left[1, \text{Re}_d^{0.077}\right] - 1}{2F(B_T)}\right), \tag{8}$$

where $B_T = \frac{c_{pv}(T_g - T_s)}{L_{\text{eff}}}$ is the Spalding heat transfer number,

$$F(B_T) = (1+B_T)^{0.7}\frac{\ln(1+B_T)}{B_T},$$

$L_{\text{eff}} = L + \frac{Q_L}{\dot{m}_d} = \sum_i \epsilon_i L_i + \frac{Q_L}{\sum_i \dot{m}_i}$, Q_L is the power spent on droplet heating, c_{pv} is the specific heat capacity of fuel vapour, $\epsilon_i = \epsilon_i(t)$ are the evaporation rates of species i, $\dot{m}_i = \epsilon_i\dot{m}_d$ ($\dot{m}_d = \sum_i \dot{m}_i$). The effects of the interaction between droplets are ignored.

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