



Modelling biodiesel droplet evaporation using continuous thermodynamics

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ABSTRACT

A model for the evaporation of droplets of biodiesel fuels based on continuous mixture theory is presented. The fuel is represented by three chemical groups – two fatty acid methyl ester (FAME) fractions and one monoglyceride fraction – and the parameters for each distribution function are derived by conducting a numerical simulation of a distillation test. Properties correlations are presented for saturated and unsaturated FAME's and for monoglycerides, and it is demonstrated that the evaporation behaviour of saturated and unsaturated FAME's is essentially identical. The model is tested against experiments on single suspended droplets and found to agree with the measurements to within 3% in d^2 .

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1. Introduction

Biodiesel fuels made from a variety of sources have been produced and extensively tested in engines. However, little work has been done on the details of the evaporation process of the droplets in a biodiesel spray. This paper applies the principles of continuous thermodynamics to develop a realistic model for the evaporation of a single droplet of biodiesel fuel and compares it with the results of experiments on suspended single droplets.

Biodiesel consists largely of fatty acid alkyl (usually methyl) esters, which are produced from the tri-glycerides in the original vegetable oil or animal fat feedstocks by transesterification with alcohols [1–3]. Small quantities of mono-, di- and tri-glycerides from partial conversion of the raw materials may also be present as well as other impurities [2,4,5]. Detailed composition information is presented by a number of authors [1,5–12], and from this it appears that most biodiesels consist of a fairly small number of esters with chains of similar length, giving a relatively flat distillation curve compared with conventional Diesel fuels [1,7–9,12–14]. Although many studies of the performance of Diesel engines fueled with biodiesel have been published [1], little has been done on the fundamentals of droplet or spray processes in biodiesel and related fuels. Pan et al. [15] have recently presented a study of single droplet combustion of biodiesel and its blends with petroleum Diesel, while Wardana [16] has reported experiments on combustion of jatropha oil droplets, the latter being the raw oil rather than the ester. A much earlier study on sunflower oil and its methyl esters was

presented by Araya and Tsunematsu [17]. Similar experiments have been done by Raghavan et al. [18] but using a porous sphere with a continuous liquid feed rather than a droplet. These papers all concentrate on single droplet combustion; however, in typical Diesel spray ignition and combustion most droplets do not burn individually, but rather evaporate inside a fairly dense spray, which then burns as a unit on its boundary. For this reason, the present paper concentrates on evaporation, rather than combustion, of biodiesel droplets.

Accurate property values are essential for modelling droplet evaporation, and a number of authors have contributed properties measurements on biodiesel fuels and related pure compounds. Several sets of vapour pressure or boiling point data for fatty acid methyl esters (FAME's) are available in the literature [1,19–28] as well as for tri-glycerides [29]. Other properties available are enthalpies of vaporization [23,25–28], liquid densities for pure compounds [24,30] and real fuels [7–9,12–14,27,32,33], liquid specific heats [31], viscosities [1,5–9,12–14,24,34,35] and thermal expansion coefficients [24,30,32,33].

2. Experiments

The procedure followed here is essentially the same as that detailed by Hallett and Beauchamp-Kiss [36]. Experiments on single droplets of 1.5–1.7 mm diameter were performed using the suspended droplet/moving furnace technique, with the apparatus being surrounded by a nitrogen atmosphere to suppress combustion and ensure pure evaporation. A single video camera continuously recorded the droplet, and droplet sizes were measured from the videos at regular intervals to track the progress of

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Nomenclature

$f(I)$	distribution function, $(\text{kg}/\text{kmol})^{-1}$	θ	mean of distribution, kg/kmol
I	distribution variable (species mol mass), kg/kmol	σ	standard deviation of distribution, kg/kmol
T	temperature, $^{\circ}\text{C}$		
Y	mass fraction		
α_p	isobaric volumetric expansion coefficient, K^{-1}	<i>Subscripts</i>	
γ	origin of distribution, kg/kmol	i	index identifying different fractions
		R	at droplet surface

evaporation. For each measurement, the major and minor diameters of the droplet were recorded and converted to an equivalent spherical diameter, assuming the droplet to be a prolate spheroid, symmetrical about the vertical axis.

Two different samples of biodiesel were used for the experiments, both produced from soybean feedstock. Distillation tests were performed on the fuel samples, and the results used to select the distribution functions for the model.

3. Numerical model

The technique of “continuous thermodynamics” represents the composition of complex multicomponent mixtures as one or more probability density functions rather than as individual species, thereby substantially reducing the number of variables that needs to be dealt with in computations. The technique has been successfully applied to fuel droplet evaporation, and the basic theory and its application to engines, mixing layers and other realistic problems have been worked out elsewhere [37–44]. It has also been applied to modelling the complexities of biofuels and alternative fuels, and successfully tested against experiments for these fuels [36,43]. The numerical model used in this paper is the same one used by Hallett and Beauchamp-Kiss [36] to model ethanol–fuel oil mixtures: it assumes quasi-steady evaporation of the droplet, and thus is not directly suited to the high pressures encountered in a diesel engine. However, the techniques and property values developed here can also be applied to continuous thermodynamics calculations at high pressure, as demonstrated by others [44].

The biodiesel fuels were modelled using three separate distribution functions to represent different fractions of the fuel: a fatty acid methyl ester (FAME) fraction comprising the bulk of the fuel, a small light FAME fraction which was found necessary to reproduce the details of the early part of the distillation curve, and a monoglyceride (MGC) fraction representing the possible presence of a small portion of partially unconverted feedstock in the fuel. Each of these is characterized by its mean θ and standard deviation σ . A gamma distribution is used to describe each group, with the origin being set to 0 in each case. For evaporation in atmospheres containing large quantities of fuel vapour it may be necessary to use a more complex function to account for the possibility of vapour condensation on the droplet in the early stages of the droplet lifetime [40,41]. It is assumed that the fuel does not contain any ethyl or higher esters; this is of course determined by the alcohol used in the production of the fuel. It is possible for mono-, di-, and tri-glycerides to be present, representing different degrees of conversion of the original oil, but detailed composition measurements by others [2,5,11] show that monoglycerides are present in much larger concentrations, typically around 0.5% compared with less than 0.1% for di- and tri-glycerides.

Both the FAME and MGC fractions were assumed to be saturated. However, biodiesels often contain large proportions of Cn:1, Cn:2 or Cn:3 unsaturated chains [6–12,35]: methyl linoleate (C18:2) in particular is present in large concentrations in many fuels, typically accounting for 51–55% of soybean biodiesel [6,7,11,12,35]. One could add a fourth group to the model to ac-

count for these. However, because the chains are fairly long, it is unlikely that the fuel properties and droplet behaviour would be changed substantially by a small degree of unsaturation. To test this assumption, properties were also developed for Cn:1 and Cn:2 FAME's, and the calculations re-run with these substituted for the main FAME fraction. As will be shown later, this made virtually no difference.

Each distribution function has two parameters – mean θ_i and standard deviation σ_i – which had to be fitted using the distillation test results together with a numerical simulation of the distillation test [36]. This meant fitting six parameters using a single curve, a task made relatively easy by the observation that each distribution controls a separate region of the distillation curve, so that the main FAME fraction could be fitted using the middle part of the curve, the light fraction using the initial 5–10%, and the unconverted MGC using the “tail”. The distribution origin γ_i was in each case assumed to be 0. Since biodiesel components are long-chain, and therefore only weakly polar, the continuous version of Raoult's law used in earlier works [37–39,43] was deemed adequate for phase equilibrium. The very good agreement shown later between theory and experiment justified this decision.

The importance of accurate property values for droplet models is often overlooked. A continuous thermodynamics model requires that properties be available in the form of fairly simple continuous functions of the distribution variable (species molecular mass in this case) so that they can be integrated during the derivation of the transport equations. The form of the correlating equations used here was as given in earlier works [37,43], and the necessary parameters for each chemical family (saturated FAME, Cn:1 and Cn:2 FAME, MGC) were generated by calculating properties for representative members of that family using standard methods [45,46] and then fitting the correlating equations to these points. More details and a list of the correlating equation parameters are given in Appendix A. In the droplet model, all vapour phase properties were assumed uniform in space but allowed to vary with time, and all were evaluated at a reference temperature and mixture composition as prescribed by Hubbard et al. [47].

4. Results

Fig. 1 shows the measured distillation curves for the two different fuel samples together with the curves produced by numerical simulation of the distillation test as described in [36]. The distribution parameters chosen for the three fractions are listed in Table 1, and the distributions for Sample 1 are illustrated in Fig. 2. The average (i.e. mean molecular mass) of the monoglyceride fraction has in each case been fixed at 60 kg/kmol higher than that of the main FAME fraction, which is equivalent to assuming that the monoglyceride and the FAME have the same average alkyl chain length. The chosen distribution functions reproduce the measurements to within an RMS error of 1.2 $^{\circ}\text{C}$. For Sample 1 alternative distribution functions were generated with Cn:1 or Cn:2 unsaturated compounds substituted for the main FAME fraction, the light FAME and MGC fractions remaining as before. These produced identical curves to the one shown in Fig. 1 when the mean of the main FAME

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