



Full Length Article

Droplet evaporation modeling of electrified fatty acid methyl esters

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ABSTRACT

The influence of electric charge on the evaporation characteristics of fatty acid methyl ester fuels from short to long carbon chain length is simulated using a validated evaporation model. A fuel droplet is assumed to undergo electrostatic fragmentation or fission in a manner which results in a large 'residual' droplet and a number of other smaller 'sibling' droplets, as has been experimentally observed in previous work. Droplet evaporation simulations are performed both for a non-reacting case and for a case where the sibling droplets burn at the adiabatic flame temperature. The simulations are complemented with measurements of biodiesel spray current taken from a charge injection atomizer, so as to enable use of experimentally measured charge as an initial condition in the simulation. Charge advantageously influences the evaporation time, particularly under the assumption that generated sibling droplets undergo combustion. The influence of charge, droplet Reynolds number and the physical properties of the methyl esters are examined, demonstrating similar overall behaviour among fuels, however showing that time histories are grouped by carbon chain length. The experimental data indicates that specific charge is a key driver behind reducing evaporation time as Reynolds number increases. However, the relationship between charge influence vs. Reynolds number diminishes in situations where sibling droplets burn. This contribution sheds light on the influence of electric charge on the vaporization of biodiesel fuels, and provides useful data which can guide future interpretation of charge influence on vaporization in reacting and non-reacting environments.

1. Introduction

Biodiesels have been suggested as an alternative to diesel fuel [3,4,9], however recent work [20] has demonstrated that biodiesels may emit a larger number of smaller nanoparticles with particle emissions increasing with an increase in the carbon chain length. Research by the same group [19] suggests that short chain fatty acid methyl esters (FAMEs) can enhance combustion efficiency in a diesel engine though resulting in higher fuel consumption. Therefore, while Biodiesels have potential to be used as a complementary resource for energy conversion, it is clear that the process of delivering and burning these fuels still requires enhancement.

As with all other plant oils, biodiesel has a higher viscosity than diesel fuel, and this can create challenges in obtaining efficient atomization. Though work on air assisted atomization has shown that in the far downstream region, biodiesel sprays have similar size distributions and dispersion characteristics [14] this is not the case in the near-field of the spray, where ligament and droplet populations are significantly different. This near-field region is of greatest relevance not only to engine applications but also to potential micro-combustion devices

where delivery in small combustion chambers necessitates very rapid atomization and vaporization over short length-scales with minimal energy consumption. This requirement necessitates precise control over dispersion as well as droplet size.

The demand for controllable injectors which can work effectively for biodiesels and other vegetable oils has driven research in electrostatic atomization [29], an atomizing technique that can work over a wide operating range (from as low as 0.5 bar injection to higher pressures of tens of bar [13,16]) with lower power consumption (2–250 mW). Electrostatic atomizers for electrically insulating liquids, also known as charge injection atomizers [29] operate through introducing an electrical charge into a bulk liquid jet such that Coulombic repulsion can assist in the liquid-fragmentation process. These devices can not only help to atomise highly viscous liquids but can also reduce the total vaporisation time of a fuel droplet [29,1]. In addition, for small engines (20–250cc), where the required pressure for generating efficient atomisation is not available, electrostatic atomisers have strong potential to offer an alternative to carburetors [15] and low pressure injectors, given that these atomizers have the proven potential to operate in transient environments [13].

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In the last three decades, considerable research has been carried out to develop charge-injection atomisers working with insulating liquids such as diesel and kerosene. The aim of increasing the spray's specific charge (charge per unit volume) has led to several modifications to nozzle design [8,25,22]. The type of electrodes, the distance between the electrode and the grounded plate, and the orifice diameter have undergone optimisation with key objectives being maximizing the spray specific charge and minimizing the amount of current lost or "leaked" to the atomiser housing [27,24,23]. However, the use of bio-fuels as a working liquid in a charge-injection atomiser has not been widely reported in the literature, though some research has been done on vegetable oils [31,1]. Research in single droplet vaporization and combustion under the influence of electric charge is more limited however the work of [2,18] has recently progressed this field through both experiments and modeling which examine the interaction between of chemi-ions and droplet charge.

In this contribution, a model previously developed and validated for the vaporization of conventional fuels [11] and electrostatic vaporization of iso-octane will be employed and enhanced to shed light on the processes that govern the atomization of an electrically charged biodiesel droplet. The model for iso-octane has been previously shown to yield good agreement with the experimental data of [2]. Initially, the model [11] is extended to account for individual fatty acid methyl ester constituents (FAME) and validated against available experimental measurements for the droplet evaporation of uncharged FAME droplets. The model is then used to examine the effect of charge on vaporization over a range of initial charge values, temperatures, and Reynolds numbers, for a range of FAMES. In a later part of the paper electrical current measurements of four different biodiesel sprays from a steady spray electrostatic atomizer are also presented and analysed. The final section presents simulation data, however makes use of the spray specific charge measurements from the biodiesel sprays as initial conditions in the evaporation simulations. Implementation of the experimental charge as an initial condition enables a more realistic interpretation of the influence of charge on vaporization in both reacting and non-reacting environments.

2. Methodology

2.1. Mathematical modelling

The full process of droplet evaporation modeling under the influence of electric charge to be used in this contribution has been recently described [11] but key features are reproduced here for the benefit of the reader. Solution of droplet temperature and mass transfer rate is achieved through equations 1 and 2 assuming uniformity across the droplet volume.

$$\frac{dT_d}{dt} = \frac{f_2 Nu}{3Pr_G} \left(\frac{\theta_1}{\tau_D} \right) (T_G - T_D) + \left(\frac{L_V}{C_L} \right) \frac{\dot{m}_d}{m_d} \quad (1)$$

$$\frac{dm_d}{dt} = - \frac{Sh}{3Sc_G} \left(\frac{m_d}{\tau_D} \right) H_M \quad (2)$$

where the droplet relaxation timescale is defined as:

$$\tau_D = \frac{\rho_D D^2}{18\mu_G} \quad (3)$$

D in Eq. (3) is the droplet diameter, ρ_D the liquid density and μ_G the gas phase viscosity.

In this contribution, a static droplet is considered, though the droplet Reynolds number ($Re = \rho_g |u_D - u_i| D / \mu_g$) may be varied through the addition of a gas phase velocity. Eq. (1) is standard and fully defined in [17] where θ_1 is the ratio of the constant pressure gas to liquid phase specific heat capacities.

In Eq. (1), T_G and T_D are the gas phase and droplet temperatures

respectively, L_V the latent heat of evaporation, C_L the liquid phase specific heat capacity, and m_d the droplet mass with ρ_D being droplet density. Dimensionless groups in equations 1 and 2 include the Nusselt number, Nu, the Prandtl number Pr_G , the Sherwood number, Sh and the Schmidt number Sc_G . H_M from Eq. (2) is calculated using an equilibrium Spalding mass-transfer number as $H_M = \ln[1 + B_{M,eq}]$ with $B_{M,eq}$ being defined in Eq. (4) and also described in [11]. The equilibrium mass fraction is determined from Eq. (5), with θ_2 being the ratio of molar masses ($\theta_2 = \frac{W_G}{W_f}$). The equilibrium mole fraction $\chi_{S,eq}$ is defined using Eq. (6) where R is the universal gas constant.

$$B_{M,eq} = \frac{Y_{S,eq} - Y_G}{1 - Y_{S,eq}} \quad (4)$$

$$Y_{S,eq} = \frac{\chi_{S,eq}}{\chi_{S,eq} + (1 - \chi_{S,eq})\theta_2} \quad (5)$$

$$\chi_{S,eq} = \frac{P_{atm}}{P_G} e^{\frac{L_V}{R} \left(\frac{1}{T_b} - \frac{1}{T_d} \right)} \quad (6)$$

For a simple equilibrium rapid mixing model (RM) f_2 from Eq. (1) is equal to unity, however as employed in previous work [11], f_2 is corrected here for the influence of evaporation on heat transfer. This is an approach as used in a Langmuir-Knudsen model [17]. Eq. (7) shows the expression defining f_2 where β is defined below, and follows the definition shown in [11] and is calculated explicitly as also noted in [17]:

$$f_2 = G = \frac{\beta}{e^{\beta} - 1} \quad (7)$$

$$\beta = - \left(\frac{3Pr_G \tau_D}{2} \right) \frac{\dot{m}_d}{m_d} \quad (8)$$

In [17,11], the wet-bulb temperature was used to calculate the properties of simple fuels like decane, hexane, and water, due to existing empirical correlations, however such correlations are not available for FAMES. Therefore, as is assumed elsewhere [30], properties here have been calculated using T_{avg} , which is the average of the gas-phase and boiling-point temperatures. This assumption is fully validated in Section 3. For a complete description of property correlations of different FAMES, the reader is directed to the Appendices of [26], which we have adopted in this contribution. All equations are solved using a 4th-order Runge-Kutta scheme. The process of accounting for charge in the vaporization of a droplet has been fully described in [11] however a brief account is provided here for the benefit of the reader.

In a charge injection atomizer, the maximum surface energy which promotes atomization is obtained from the mutual repulsion of net charges which are accumulated on the whole or partial surface of the droplets [31]. A single droplet with a diameter D [m] can hold a maximum surface charge given by Eq. (9) [21]:

$$Q_{ray} = \pi (\epsilon\sigma)^{1/2} (2D)^{3/2} \quad (9)$$

where ϵ is the permittivity of vacuum [F/m], σ is the surface tension [N/m] and Q_{ray} in Eq. (9) is known as the Rayleigh limit. Through the vaporization process, the droplet diameter decreases, and as its volume weighted charge approaches the Rayleigh limit, fragmentation occurs. In practice, individually charged droplets usually break up well below the Rayleigh limit [31] and therefore the fragmentation limit can be rewritten as follows:

$$Q_{ray} = \eta (\pi (\epsilon\sigma)^{1/2} (2D)^{3/2}) \quad (10)$$

where η is the Rayleigh limit coefficient ($\eta \leq 1$), typically equal to 0.8 in this contribution unless otherwise specified. As a droplet fragments due to electrostatic charge, it separates into a larger residual droplet and into an n number of smaller sibling droplets as schematically shown in Fig. 1. In the case of no chemical reaction, this residual droplet evaporates using the evaporation model described above. Based on previous studies [11] it is assumed that after fragmentation, the

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