Modelling of droplet heating and evaporation: an application to biodiesel, gasoline and Diesel fuels

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Abstract

This paper presents our recent progress in the modelling of automotive fuel droplet heating and evaporation processes in conditions close to those in internal-combustion engines. Three types of automotive-fuels are considered: biodiesel, gasoline and Diesel fuels. Modelling of biodiesel fuel droplets is based on the application of the Discrete Component (DC) model. A distinctive feature of this model is that it is based on the analytical solutions to the transient heat conduction and species diffusion equations in the liquid phase, taking into account the effects of recirculation. The application of the DC model to fossil fuels (containing potentially hundreds of components), however, is computationally expensive. The modelling of these fuels is based on the recently introduced Multi-Dimensional Quasi-Discrete (MDQD) model. This model replaces large number of components in Diesel and gasoline fuels with a much smaller number of components/quasi-components without losing the main features of the original DC model. The MDQD model is shown to accurately predict the droplet temperatures and evaporation times and to be much more computationally efficient than the DC model. The main features of these models and their applications to automotive fuel droplets are summarised and discussed.

Keywords: Automotive fuel, Droplet, Heating, Evaporation, Modelling, Multi-component.

1. Introduction

Studies of the heating and evaporation of automotive fuel droplets are crucial to the design of internal combustion engines and ensuring their good performance [1–5]. Possible approaches to modelling these processes have been discussed by many authors including [6–9]. The models discussed in these papers, however, are based on several crude assumptions, which are required either to reduce the complexity of the models or to adapt the models to limited applications. The most important of these assumptions are that: 1) multi-component automotive fuels can be approximated by single components (e.g. n-dodecane is used to represent Diesel fuel and iso-octane is used to represent gasoline fuel); 2) temperature gradients inside the droplets can be ignored (using the Infinite Thermal Conductivity (ITC) model); 3) recirculation due to relative droplet and gas velocities can be ignored; or 4) the diffusion of species inside the droplets is either ignored or assumed to be infinitely fast (using the Infinitely fast Diffusivity (ID) model). These effects have been taken into account in a series of our recently developed models [10–15]. In this paper these models are briefly described and some results of their application to automotive fuel droplets are summarised.

Biodiesel fuels are mainly composed of relatively small numbers (6 to 17) of fatty acid ethyl and methyl esters [15,16,17-20]. This allows us to apply directly the Discrete Component (DC) model to modelling biodiesel fuel droplet heating and evaporation (see [11,12,15]). In the case of fossil fuels (containing possibly hundreds of components), the DC model is computationally very expensive when directly applied to modelling droplet heating and evaporation. In response to this problem, the Multi-Dimensional Quasi-Discrete (MDQD) model has been developed. In this model, a large number of components in realistic automotive fuels is replaced with a small number of quasi-components, taking into account the same effects as considered in the DC model [14]. This model has been shown to accurately predict the temperature of droplets and their evaporation times and to be computationally efficient (see [10,12,14]). Some results of applications of the above-mentioned models are briefly summarised in Section 2.

2. Results

In this paper, the analysis of biodiesel fuel droplets, based on the DC model, focuses on Palm Kernel Methyl Ester (PME). The molar fractions of the pure fatty acids contributing to PME are inferred from the data reported in [18,19]. As mentioned in Section 1, in the case of gasoline and Diesel fuels, the DC model is computationally expensive. Hence, the MDQD model is used for the analysis of heating and evaporation of these fuels (see [14] for the details of this model).

In all cases, calculations have been performed using the following models: 1) the ETC/ED model taking into account the contributions of all components of automotive fuel (ME model); 2) a model in which the transport and thermodynamic properties are averaged, ignoring the diffusion of species and assuming that liquid thermal conductivity is infinitely large (SI model). In the cases of

gasoline and Diesel fuels, the above-mentioned MDQD model has been used alongside the SI model.

Our preliminary results show that the approximations of the above-mentioned automotive fuels with single-component fuels lead to under-prediction of droplet evaporation times by about 26% for biodiesel fuel droplets, 50% for Diesel fuel droplets, and 47% for gasoline fuel droplets, which are not acceptable in most engineering applications. Also, it has been found that the approximation of 98 components of Diesel fuel with 15 components/quasi-components leads to under-prediction of evaporation time by less than 2.5%, which can be acceptable in most engineering applications. This has also reduced CPU time to 1/6th compared with the case when all 98 components are taken into account.

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