Modelling of automotive fuel droplet heating and evaporation: recent results and unsolved problems

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Abstract

Recent results of the investigation of automotive fuel droplet heating and evaporation are summarised. The results of calculations of heating and evaporation of biodiesel fuel droplets, taking into account the contributions of all components, using the discrete component models with finite and infinitely small species diffusivities are discussed. It is pointed out that there are serious problems with the application of the Discrete Components Model, based on the analysis of diffusion of individual components, to the modelling of heating and evaporation of realistic Diesel fuel droplets. Some results of the development of the generalised multi-dimensional quasi-discrete model and its application to realistic Diesel fuel droplets are presented. New approaches, based on kinetic and molecular dynamics models, are briefly summarised. The effects of inelastic collisions and the presence of several components in automotive fuel on the results of kinetic modelling are investigated. The molecular dynamics models used for the estimation of the evaporation/condensation coefficient for n-dodecane droplets ($C_{12}H_{26}$) are based on the assumption that the C–H bond in complex hydrocarbon molecules, such as n-dodecane, is much shorter and much stronger than the C–C bond, and also stronger than the van der Waals forces between molecules. Thus the methyl (CH_3) or methylene (CH_2) groups can be regarded as separate atom-like structures in a relatively simple United Atom Model. Some results of the application of quantum chemical methods to the estimation of this coefficient are discussed. The most important unsolved problems are identified.

Keywords: Automotive fuel, Droplet, Heating, Evaporation, Kinetic models, Molecular dynamics models, Multi-component.

1. Introduction

The problem of modelling heating and evaporation of automotive fuel droplets is a long standing one, and has been discussed in many papers, some results of which are summarised in [1]. The most widely used engineering approach to modelling the above processes is based on the direct application of one of the commercial or research computational fluid dynamics codes. Without questioning the need for such an approach, the main emphasis of the authour's research has been on different problems. These include the investigation of the underlying physics of the processes involved, and development of the new physical and mathematical models of the processes. This 'physical' approach to the modelling of droplets is not expected to replace the conventional 'engineering' approach but is expected to complement it. The main objective of this abstract is to give an overview of the most important new models and results concerning automotive fuel droplet heating and evaporation presented by the author and his colleagues.

2. Models

In most commercial and research computational fluid dynamics codes the modelling of droplet heating and evaporation is based on the assumptions that there is no temperature gradient inside droplets and kinetic effects can be ignored. In the case of multi-component droplets, the species diffusivity within the droplet is assumed to be infinitely large or small [1]. New approaches to numerical modelling of droplet heating and evaporation by convection and radiation from the surrounding hot gas were suggested and discussed in a number of our earlier papers the results of which are summarised in [1]. In these approaches, the finite thermal conductivity of liquid fuel and recirculation within droplets were taken into account. These approaches were based on the incorporation of the new analytical solution to the heat conduction equation inside the droplets into numerical codes. This solution was applied to the first time step, using the initial distribution of temperature inside the droplet. The results of the analytical solution over this time step were used as the initial condition for the second time step. The relatively small contribution of thermal radiation to droplet heating and evaporation led to the suggestion that the variations of radiation absorption inside droplets can be ignored. In [2,3] a new model, taking into account the effect of the moving interface on droplet heating and evaporation, is suggested. The authors of [2] assumed that the droplet radius is a linear function of time during individual time steps, while in [3] it was assumed that the time evolution of droplet radius $R_d(t)$ is known. For sufficiently small time steps the time evolutions of droplet temperatures and radii predicted by both approaches coincided. The predictions of the model developed in [2] were also shown to be in agreement with the results reported in [4], based on the direct numerical solution of the heat conduction equation inside droplets.

A model for multi-component droplet heating and evaporation, taking into account all key processes, including the distribution of temperature and diffusion of liquid species inside the droplet and the effects of the non-unity activity coefficient was developed in [5]. The

previously obtained analytical solution to the transient heat conduction equation inside droplets was incorporated into the numerical code alongside the new analytical solution to the species diffusion equation inside droplets. This model, taking into account the effect of diffusion of individual species inside the droplets, is widely known as the Discrete Component Model (DCM).

The effects of the moving interface on droplet heating and evaporation, taking into account both heat conduction and species diffusion, were investigated in [6,7]. These effects were shown to be much stronger for the solution to the species diffusion equation than for the solution to the heat conduction equation.

A quasi-discrete model for heating and evaporation of complex multi-component hydrocarbon fuel droplets was suggested and tested in Diesel engine-like conditions [8,9]. The original version of this model is applicable to the case when the fuel can be approximated by *n*-alkanes, C_nH_{2n+2}, characterised by carbon numbers *n*. The components with relatively close *n* were replaced by quasi-components with properties calculated as average properties of *a priori* defined groups of actual components. The analysis of heating and evaporation of droplets consisting of many components was replaced by the analysis of heating and evaporation of droplets consisting of relatively few quasi-components. The effects of temperature gradient and quasi-component diffusion inside droplets were taken into account. In [10] the quasi-discrete model was generalised to take into account the components other than alkanes. The generalised version of the quasi-discrete model was called the multi-dimensional quasi-discrete (MDQD) model.

All above-mentioned models were generalised to be applicable to moving droplets, using the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model in which liquid thermal conductivity and diffusivity were replaced by effective liquid thermal conductivity and diffusivity.

The analysis in the above-mentioned papers was implicitly based on the assumption that both liquid and gas phases can be treated as a continuum. The validity of this assumption is not obvious in the immediate vicinity of the interface between liquid droplets even in the case when pressure is well above 1 atm [1]. This means that the properties of gas in the vicinity of the liquid-gas interface can depend not only on the average velocities of molecules, but also on the distribution of molecules in terms of velocities. The latter is generally described in terms of distribution functions, studied by kinetic models [1].

In the approach developed in a series of our early papers, summarised in [1], two regions of gas above the surface of the evaporating droplet were considered: the kinetic (about 10-50 mean molecular paths thick) and hydrodynamic regions. The analysis of the processes in the kinetic region was based on the numerical solution to the Boltzmann equations for fuel vapour (approximated by n-dodecane) and background gas (approximated by nitrogen) with relevant boundary conditions at the droplet surface and interface between the kinetic and hydrodynamic regions. These models were generalised in [11,12] to take into account the effects of inelastic collisions between molecules in the kinetic region. In the new model the effect of inelastic and elastic collisions was described as a random rotation of the *N*-dimensional vector in the *N*-dimensional space, without specifying the physical nature of the inelastic collisions. It was shown that for any given temperature at the outer boundary of the kinetic region the values of the heat flux decrease with increasing numbers of internal degrees of freedom of the molecules. The rate of this decrease was strong for small numbers of these degrees, but negligible when their number exceeded 20. This allowed the authors to restrict the analysis to the first 20 arbitrarily chosen degrees of freedom when considering the effects of inelastic collisions. In [13] these models were further generalised to take into account the presence of three components in the kinetic region (n-dodecane and p-dipropylbenzene, approximating Diesel fuel, and nitrogen, approximating air).

The above-mentioned kinetic models rely on the value of the evaporation coefficient. A commonly used approach to estimating this coefficient is based on the molecular dynamics analysis in the immediate vicinity of the liquid gas interface. In [14,15], this analysis was used to study the evaporation and condensation of n-dodecane ($C_{12}H_{26}$). The interactions in molecular structures were modelled using the United Atom Model. In this model, the methyl (CH_3) or methylene (CH_2) groups are regarded as separate atom-like structures (see [14,15] for the details). More advanced models, taking into account quantum chemical effects, are discussed in [16,17].

3. Results

In this section, some key results of the applications of the models described in Section 2 are summarised. In [18] biodiesel fuel droplet heating and evaporation was investigated using the models described in Section 2. The temperature gradient, recirculation, and species diffusion within droplets were taken into account. Calculations were 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 was pointed out that for all types of biodiesel fuel considered in this paper the predictions of the multi-component and single component models were rather close (the droplet evaporation times predicted by these models differed by less than about 5.5%).

The multi-dimensional quasi-discrete model, mentioned in Section 2, was tested for the analysis of heating and evaporation of realistic Diesel fuel droplets. In this model quasi-components were formed within individual groups. In contrast to the original quasi-discrete model, the contributions of individual components were not approximated by the distribution function of carbon numbers. The formation of quasi-components was based on taking into account the contributions of individual components without any approximations. Groups contributing small molar fractions to the composition of Diesel fuel (less than about 1.5%) were replaced with characteristic components. Six groups (alkanes, cycloalkanes, bicycloalkanes, alkylbenzenes, indanes & tetralines, and naphthalenes) and 3 components (tricycloalkane, diaromatic and phenanthrene) were identified in the fuel. It was shown that the approximation of Diesel fuel by 15 quasi-components and components, leads to errors in estimated temperatures and evaporation times in typical Diesel engine conditions not exceeding about 3.7% and 2.5% respectively.

In the model used in [19] the presence of two components in the vapour (n-dodecane and p-dipropylbenzene), finite thermal conductivity and finite species diffusivity in droplets were taken into account. The model was tested for the analysis of heating and evaporation of a droplet with initial radius and temperature equal to 5 μm and 300 K, respectively, immersed into gas with temperatures 1000 K and 700 K. It was shown that an increase in the mass fraction of p-dipropylbenzene and kinetic effects leads to an increase in the predicted droplet evaporation time.

In [14,15] it was shown that the evaporation/condensation coefficient, estimated using the MD approach based on the United Atom Model, decreases with increasing temperatures, and its values were shown to be close to those predicted based on other approaches. As shown in [16], these values are also close to those calculated taking into account quantum chemical effects.

Although the above-mentioned results show considerable progress in the development of the models for automotive fuel droplet heating and evaporation, there are still a number of issues which are not yet fully resolved. All of the above-mentioned models are based on the assumption that droplets are spherical, and they rely heavily on the assumption that the ETC/ED model is valid (the range of validity of this model has never been thoroughly investigated). The effects of interactions between droplets, largely ignored in our analysis, can be dominant in realistic engine applications. The kinetic algorithms, described above, cannot be incorporated directly into computational fluid dynamics codes. Efficient approximation of the kinetic results would be essential to taking into account the kinetic effects in these codes. All of these issues are discussed in more detail in [20].

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References

[1] Sazhin SS. Droplets and Sprays. London: Springer; 2014.

[2] Sazhin SS, Krutitskii PA, Gusev IG, Heikal M. Transient heating of an evaporating droplet, Int. J Heat Mass Transfer 2010;53:2826–36

[3] Sazhin SS, Krutitskii PA, Gusev IG, Heikal M. Transient heating of an evaporating droplet with presumed time evolution of its radius, Int. J Heat Mass Transfer 2011;54:1278–88.

[4] Mitchell SL, Vynnycky M, Gusev IG, Sazhin SS. An accurate numerical solution for the transient heating of an evaporating spherical droplet, Applied Mathematics and Computation 2011;217:9219–33.

[5] Sazhin SS, Elwardany A, Krutitskii PA, Castanet G, Lemoine F, Sazhina EM, et al. A simplified model for bi-component droplet heating and evaporation, Int J Heat Mass Transfer 2010;53:4495–505.

[6] Gusev IG, Krutitskii PA, Sazhin SS, Elwardany A. A study of the species diffusion equation in the presence of the moving boundary, Int. J Heat Mass Transfer 2012;55:2014–21.

[7]. Elwardany AE, Gusev IG, Castanet G, Lemoine F, Sazhin SS. Mono- and multi-component droplet cooling/heating and evaporation: comparative analysis of numerical models, Atomization and Sprays 2011;21:907–31.

[8] Sazhin SS, Elwardany A, Sazhina EM, Heikal MR. A quasi-discrete model for heating and evaporation of complex multicomponent hydrocarbon fuel droplets, Int. J of Heat Mass Transfer 2011;54:4325–32.

[9] Elwardany AE, Sazhin SS. A quasi-discrete model for droplet heating and evaporation: application to Diesel and gasoline fuels, Fuel 2012;97:685–94.

[10] Sazhin SS, Al Qubeissi M, Nasiri R, Gun'ko VM, Elwardany AE, Lemoine F, Grisch F, Heikal MR.. A multi-dimensional quasi-discrete model for the analysis of Diesel fuel droplet heating and evaporation, Fuel 2014;129:238–66.

[11] Sazhin SS, Xie J-F, Shishkova IN, Elwardany AE, Heikal MR. A kinetic model of droplet heating and evaporation: effects of inelastic collisions and a non-unity evaporation coefficient, Int. J Heat Mass Transfer 2013; 56:525–37.

[12] Shishkova IN, Sazhin SS, Xie J-F. A solution of the Boltzmann equation in the presence of inelastic collisions, J Computational Physics 2013;232:87-99.

[13] Shishkova IN, Sazhin SS. A solution of the Boltzmann equation in the presence of three components and inelastic collisions. Int J of Heat and Mass Transfer 2014; 71:26-34.

[14] Cao B-Y, Xie J-F, Sazhin SS. Molecular dynamics study on evaporation and condensation of *n*-dodecane at liquid-vapour phase equilibria, J Chemical Physics 2011;134:164309.

[15] Xie J-F, Sazhin SS, Cao B-Y. Molecular dynamics study of the processes in the vicinity of the *n*-dodecane vapour/liquid Interface, Physics Fluids 2011;23:112104.

[16] Gun'ko, VM, Nasiri R, Sazhin SS. A study of the evaporation and condensation of *n*-alkane clusters and nanodroplets using quantum chemical methods, Fluid Phase Equilibria 2014;366:99-107.

[17] Gun'ko, VM, Nasiri R, Sazhin SS. Effects of the surroundings and conformerisation of *n*-dodecane molecules on evaporation/condensation processes. J Chemical Physics 2015 (in press).

[18] Sazhin SS, Al Qubeissi M, Kolodnytska R, Elwardany A, Nasiri R, Heikal MR. Modelling of biodiesel fuel droplet heating and evaporation, Fuel 2014;115:559-72

[19] Sazhin SS, Shishkova IN, Al Qubeissi M. Heating and evaporation of a two-component droplet: hydrodynamic and kinetic models. Int J Heat Mass Transfer 2014;79:704-12.

[20] Sazhin SS, Heikal MR. Droplet heating and evaporation - recent results and unsolved problems, Computational Thermal Sciences 2012;4:485-96.