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Review article

# Modelling of fuel droplet heating and evaporation: Recent results and unsolved problems

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The most recent developments in the modelling of heating and evaporation of fuel droplets, the results of which were published in 2014–2017, are reviewed, and the most important unsolved problems are identified. Basic principles of power law and polynomial approximations and the heat balance method for modelling the heating of non-evaporating droplets are discussed. Several approaches to modelling the heating of evaporating droplets, predicting different heating and evaporation characteristics, are compared. New results in modelling heating and evaporation of spheroidal droplets are identified. Basic principles of the Discrete Component Model and its application to biodiesel fuel droplets are summarised. Main ideas of the Multi-dimensional Quasi-discrete Model and its applications to Diesel and gasoline fuel droplets are discussed. New developments in gas phase evaporation models for multi-component fuel droplets are presented. A self-consistent kinetic model for droplet heating and evaporation is described. New approaches to the estimation of the evaporation coefficient, including those taking into account quantum-chemical effects, are summarised. Among unsolved problems, the effects of non-spherical droplets, limitations of the ETC/ED model, effects of the interaction between droplets, effects of the moving interface due to evaporation, modelling of complex multi-component droplets, modelling of droplet heating and evaporation in near- and super-critical conditions, development of advanced kinetic and molecular dynamics models and effective approximation of the kinetic effects are discussed.



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## 1. Introduction

The modelling of droplet heating and evaporation has been extensively studied since the beginning of the last century, and the results of these studies have been summarised in numerous reviews and monographs including those published by the author [1,2]. The main stimulus for these studies has been linked with engineering, environmental and pharmaceutical applications of the results of this modelling. For example, droplet heating and evaporation is an integral part of the processes leading to autoignition of the automotive fuel vapour/air mixture in Diesel engines [3]. The scope of the present review is more limited compared with most previously published reviews and monographs, including [1,2]. It will focus primarily on the modelling of automotive fuel droplets (although some results may have a much wider range of application) and results not included in monograph [2] (although there will be some overlap with the results presented in this monograph; on some occasions the same topics as in [2] will be considered but using different approaches from those described in [2]). As in [1,2], some topics related to droplet heating and evaporation will not be covered in this review, including heating and evaporation of droplets during their interaction with walls and the Soret effect (see [4] for a recent review of the latter phenomenon). The analysis of purely experimental papers focused on the study of droplet heating and evaporation and papers focused on multi-dimensional simulations of heated and evaporating sprays will be very limited. This review is intended to be complementary to recently published reviews [5,6], where the main focus is on ignition and combustion of individual droplets and arrays of droplets, rather than fuel droplet heating and evaporation.

The overall structure of the review is similar to that of [1,2]. The approaches to modelling of non-evaporating droplets are reviewed in Section 2. The models for droplet heating and evaporation of mono-component droplets are discussed in Section 3. The heating and evaporation models for more realistic multi-component droplets are reviewed in Section 4. Section 5 focuses on kinetic and molecular dynamics models. The main unsolved problems are summarised and discussed in Section 6.

## 2. Heating of non-evaporating droplets

This section consists of two parts. Firstly the models described in [2] will be briefly summarised with some of the most recent relevant references added. Secondly, the discussion will focus on new models, not previously described in [2].

### 2.1. Background research into modelling the heating of non-evaporating droplets

In this subsection the models for heating of non-evaporating droplets, described in [2], are briefly summarised. The original references, mentioned in [2], will not be reproduced in most cases, but relevant new references will be added. Since most of the material presented in this section is described in detail in [2], references to this monograph will be omitted in most cases. As in [1,2], the models for convective and radiative heating will be described separately.

#### 2.1.1. Convective heating of non-evaporating droplets

The most widely used model for droplet heating, for both non-evaporating and evaporating droplets, is the one based on the assumption that liquid thermal conductivity is infinitely large. This model predicts that there is no temperature gradient inside droplets and the evolution of droplet temperature with time is inferred from the energy balance equation: all heat transferred from the ambient gas is spent on raising droplet temperature. Despite the simplicity of this model, it is almost universally used in research and commercial Computational Fluid Dynamics (CFD) and many original investigations of the problem of droplet heating, including the most recent ones (see Section 3.1).

In the case of stationary spherical droplets, the effects of temperature gradient within them were taken into account based on the solution to the one-dimensional (1D) heat transfer equation, assuming that the heating process is also spherically symmetric. This equation was solved either numerically (e.g. [7]) or analytically (see [2]). Two types of boundary conditions at the surface of the droplet were considered. Firstly, these were Robin boundary