



# Heating and evaporation of a two-component droplet: Hydrodynamic and kinetic models



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## ABSTRACT

A previously developed kinetic model for two-component vapour and background gas (air) is applied to the analysis of droplet heating and evaporation in Diesel engine-like conditions. The model used in the analysis is based on the introduction of the kinetic region in the immediate vicinity of the droplets and the hydrodynamic region. The presence of two components in the vapour, finite thermal conductivity and finite species diffusivity in droplets are taken into account. It is pointed out that for parameters which are typical of Diesel engine-like conditions, the heat flux in the kinetic region is a linear function of the temperature at the outer boundary of this region, but is almost independent of the density of the components at this boundary. Mass fluxes of both components in the kinetic region are shown to decrease almost linearly with increasing vapour density at the outer boundary of this region, but are almost independent of the temperature drop in the kinetic region. The model is tested for the analysis of heating and evaporation of a droplet with initial radius and temperature equal to 5  $\mu\text{m}$  and 300 K, respectively, immersed into gas with temperatures 1000 K and 700 K for several mixtures of n-dodecane and p-dipropylbenzene. It is pointed out that an increase in the mass fraction of p-dipropylbenzene and kinetic effects lead to an increase in the predicted droplet evaporation time. The kinetic effects are shown to increase with increasing gas temperature and molar fraction of p-dipropylbenzene.

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## 1. Introduction

An interest in modelling droplet heating and evaporation has been stimulated by various engineering, environmental and pharmaceutical applications [1,2]. In most engineering applications, including automotive ones, the modelling of these processes has been based on the hydrodynamic approximation, although the limitations of this approximation, even in the case when these processes take place at high pressures, are well known (see [3–5]). In a number of studies, including [6–9], the evaporation of n-dodecane  $\text{C}_{12}\text{H}_{26}$  (an approximation for Diesel fuel) was studied and a new model was developed based on a combination of the kinetic and hydrodynamic approaches. In the immediate vicinity of droplet surfaces (up to about one hundred molecular mean free paths), the vapour and ambient gas dynamics were studied based on the Boltzmann equation (kinetic region), while at larger distances the analysis was based on the hydrodynamic equations (hydrodynamic

region). Mass, momentum and energy fluxes were conserved at the interface between these regions. The authors of [7–9] considered the problem of n-dodecane evaporation into air and developed a new numerical algorithm for the solution of a system of two Boltzmann equations for n-dodecane and air, taking into account elastic collisions between: n-dodecane molecules; between air molecules; and between n-dodecane and air molecules. A new approach to taking into account the effects of inelastic collisions was developed in [10] and applied to the problem of n-dodecane droplet heating and evaporation in [11].

One of the important limitations of the approaches described in [6–11] is that they were based on the assumption that Diesel fuel can be approximated by n-dodecane. A more detailed analysis of the composition of Diesel fuel showed that it includes hundreds of various hydrocarbon components [12–14]. It is obviously not possible to take into account the contributions of all these components in the kinetic modelling. At the same time, one can see that these components can be subdivided into two main groups: alkanes and aromatics [14]. The assumption that n-dodecane can approximate alkanes is widely used (see [12,15,16]), while aromatics could be approximated by p-dipropylbenzene [15]. In this case

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**Nomenclature**

$B_M$	Spalding mass transfer number
$B_T$	Spalding heat transfer number
$c$	specific heat capacity
$D$	binary diffusion coefficient
$f$	molecular velocity distribution function
$E$	relative error defined by Eq. (18)
$h$	convection heat transfer coefficient
$j$	mass flux
$J$	collision integral
$k$	thermal conductivity
$\ell$	mean free path
$L$	latent heat of evaporation
$Le$	Lewis number
$m$	mass
$M$	molar mass
$N_{at}$	the total number of atoms in a molecule
$Nu$	Nusselt number
$p$	pressure
$Pr$	Prandtl number
$q$	heat flux
$Q_L$	power spent on droplet heating
$\mathbf{r}$	radius-vector
$R$	distance from the centre of the droplet
$R_{v(a)}$	gas constant referring to n-dodecane (air)
$R_d$	droplet radius
$Sc$	Schmidt number
$T$	temperature
$\mathbf{v}$	velocity
$X$	molar fraction
$Y$	mass fraction

**Greek symbols**

$\alpha$	parameter defined by Eq. (6)
$\beta$	evaporation coefficient

$\delta_{Rd}$	thickness of the kinetic region
$\epsilon_i$	evaporation rate of individual species
$\theta$	angular coordinate
$\kappa$	liquid diffusivity
$\rho$	density
$\sigma$	effective diameter of molecules
$\phi$	angular coordinate

**Subscripts**

$a$	air
$at$	atom
$\alpha, \beta$	$\alpha = a, n, p; \beta = a, n, p$
$d$	droplet
$eff$	effective
$g$	gas
$h$	hydrodynamic
$i$	components
$k$	kinetic
$l$	liquid
$n$	n-dodecane
$p$	constant pressure or p-dipropylbenzene
$r$	reference or reflected
$Rd$	outer boundary of the kinetic region
$s$	surface
$total$	total
$v$	fuel vapour
$0$	initial
$\infty$	ambient

**Superscripts**

$i$	components
$'$	after the collision
$\sim$	normalised

it was suggested that a more accurate approximation of Diesel fuel, compared with the one based on its approximation by n-dodecane, could be its approximation by a mixture of n-dodecane and p-dipropylbenzene. Mass fractions of n-dodecane in this mixture could vary from 0.8 to 0.7 [15,12].

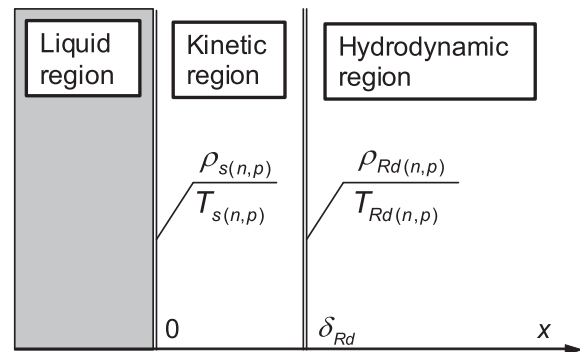
A new kinetic algorithm for modelling of a three component (two components, approximating Diesel fuel, and air, approximated by nitrogen) mixture was developed in [17]. Binary collisions between molecules were taken into account assuming that these collisions are elastic or inelastic. The functionality testing of the algorithm was performed using a simple test problem of heat and mass transfer in a mixture of n-dodecane, p-dipropylbenzene and nitrogen between two infinite parallel walls. It was concluded that the predictions of the new kinetic algorithm are qualitatively consistent with the predictions of more basic models of the phenomena for which it was tested.

The aim of this paper is to investigate the kinetic effects on heating and evaporation of two-component droplets, approximating Diesel fuel, assuming that this approximation is a mixture of n-dodecane and p-dipropylbenzene. The numerical algorithm developed in [17] will be used in our analysis.

The mathematical model, used in the analysis, is discussed in Section 2. In Section 3 this model is applied to the analysis of heating and evaporation of a two-component (mixture of n-dodecane and p-dipropylbenzene) droplet. The results are compared with those based on the approximation of Diesel fuel droplets by n-dodecane droplets. The main results of the paper are summarised in Section 4.

**2. Mathematical models**

As in [6–11], two regions above the surface of an evaporating fuel droplet are considered: the kinetic and hydrodynamic regions. As in [11], we take into account that thermal conductivity of the liquid phase is finite, and identify the third region called the liquid phase region. All three regions are schematically shown in Fig. 1.  $T_s$  and  $\rho_{s(n,p)}$  refer to the surface temperature and vapour density (for



**Fig. 1.** Liquid, kinetic and hydrodynamic regions near the surface of the droplet.  $T_s$  is the droplet surface temperature,  $\rho_{s(n,p)}$  are the n-dodecane ( $n$ ) and p-dipropylbenzene ( $p$ ) vapour densities in the immediate vicinity of the droplet surface,  $T_{Rd}$  and  $\rho_{Rd(n,p)}$  are the temperature and the n-dodecane ( $n$ ) and p-dipropylbenzene ( $p$ ) vapour densities at the outer boundary of the kinetic region.

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