

A self-consistent kinetic model for droplet heating and evaporation

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Abstract

A new kinetic model for heating and evaporation of Diesel fuel droplets is suggested. The model is based on the introduction of the kinetic region in the immediate vicinity of the heated and evaporating droplets, where the dynamics of molecules are described in terms of the Boltzmann equations for vapour components and air, and the hydrodynamic region. The effects of finite thermal conductivity and species diffusivity inside the droplets and inelastic collisions in the kinetic region are taken into account. Diesel fuel is approximated by n-dodecane or a mixture of 80% n-dodecane and 20% p-dipropylbenzene. In both cases, the evaporation coefficient is assumed equal to 1. The values of temperature and vapour density at the outer boundary of the kinetic region are inferred from the requirement that both heat flux and mass flux of vapour (or vapour components) in the kinetic and hydrodynamic regions in the vicinity of the interface between these regions should be equal. Initially, the heat and mass fluxes in the hydrodynamic region are calculated based on the values of temperature and vapour density at the surface of the droplet. Then the values of temperature and vapour density at the outer boundary of the kinetic region, obtained following the above-mentioned procedure, are used to calculate the corrected values of hydrodynamic heat and mass fluxes. The latter in their turn lead to new corrected values of temperature and vapour density at the outer boundary of the kinetic region etc. It is shown that this process quickly converges for the cases analysed in the paper, and it leads to self-consistent values for both heat and mass fluxes. The model is applied to the analysis of heating and evaporation of Diesel fuel droplets with initial radii and temperature equal to 5 μm and 300 K, immersed into gas with temperatures in the range 800-1200 K and pressure equal to 30 bar. It is shown that in all cases the kinetic effects lead to a decrease in droplet surface temperature and an increase in the evaporation time. The kinetic effects on the droplet evaporation time are shown to increase with increasing gas temperatures.

Keywords: Boltzmann equation, Diesel fuel droplet, n-dodecane, p-dipropylbenzene, heat/mass transfer, kinetic effects

Nomenclature

B_M	Spalding mass transfer number
B_T	Spalding heat transfer number
c	specific heat capacity
D	binary diffusion coefficient
E	relative error defined by Equation (13)
F	parameter defined by Equation (9)
h	convection heat transfer coefficient
j	mass flux
k	thermal conductivity
L	latent heat of evaporation
Le	Lewis number
m	mass
Nu	Nusselt number
p	pressure
Pr	Prandtl number
q	heat flux
Q_L	power spent on droplet heating
Re	Reynolds number
R_v	gas constant referring to n-dodecane
R_d	droplet radius
Sc	Schmidt number
Sh	Sherwood number
T	temperature
Y	mass fraction

Greek symbols

α_ρ, α_T	$\rho_{Rd}/\rho_s, T_{Rd}/T_s$
δ_{Rd}	thickness of the kinetic region
ϵ_i	evaporation rate of individual species
ρ	density
φ	parameter defined by Equation (8)

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Subscripts

a	air
cr	critical
d	droplet
e	evaporation
eff	effective
g	gas
h	hydrodynamic
i	components
k	kinetic
mix	mixture
n	n-dodecane
p	constant pressure or p-dipropylbenzene
r	reference
Rd	outer boundary of the kinetic region
s	surface
v	fuel vapour
0	initial
∞	ambient

Superscripts

i	components
sat	saturated
\sim	normalised

1. Introduction

In most engineering applications, including automotive ones, the modelling of droplet heating and evaporation processes has been based on the hydrodynamic approximation, when vapour at the droplet surface is assumed to be saturated and the problem of droplet evaporation reduces to the problem of diffusion of vapour from the droplet surface to the ambient gas [1]. At the same time, the limitations of this approximation, even in the case when these processes take place at high pressures, have been well known since

7 the pioneering papers published more than 100 years ago (see the references in [2]). In a number of stud-
8 ies, including [3]-[8], the evaporation of n-dodecane $C_{12}H_{26}$ (an approximation for Diesel fuel) was studied
9 and a new model combining the kinetic and hydrodynamic approaches was developed. In the immediate
10 vicinity of droplet surfaces (up to about one hundred molecular mean free paths), the vapour and ambient
11 gas dynamics were studied based on the Boltzmann equations for vapour and air (kinetic region), while
12 at larger distances the analysis was based on the hydrodynamic equations (hydrodynamic region). Mass,
13 momentum and energy fluxes were conserved at the interface between these regions. In [9, 10] this approach
14 was generalised to take into account the contribution of two components in liquid and vapour. Using this
15 method, Diesel fuel was approximated as a mixture of n-dodecane (approximating alkanes in Diesel fuel)
16 and p-dipropylbenzene (approximating aromatics in Diesel fuel). The modelling took into account the con-
17 tributions of three components in the kinetic region (two components approximating Diesel fuel, and air
18 approximated by nitrogen).

19 In all of the above-mentioned kinetic models it was assumed that the distribution function of evaporated
20 molecules is Maxwellian and vapour pressure at the droplet surface is saturated (mono-component droplets)
21 and obeys Raoult's law (bi-component droplets). The mass flux of evaporated molecules was controlled by
22 the evaporation coefficient, which is the ratio of the actual mass flux of molecules leaving the droplet surface
23 and the maximal possible one. In the earliest publication [3] this coefficient was assumed to be equal to
24 0.04 and 0.5 (minimal and average values of this coefficient for water). Later, it was assumed equal to 1,
25 except in [8]. In the analysis presented in [8] the values of this coefficient inferred from molecular dynamic
26 simulations of the evaporation of n-dodecane [11] were used. The analysis presented in [11] was based on
27 the so called Force Field (FF) approximation, when quantum mechanics effects due to the contribution of
28 electron shells were not taken into account. Later it was shown that quantum mechanics effects do not have
29 significant influence on the values of this coefficient [12, 13]. As shown in our previous papers (e.g. [8]) the
30 effect of the evaporation coefficient on the droplet evaporation rate is relatively small. In our analysis this
31 coefficient is assumed to be equal to 1.

32 In all models described in [3]-[8] and [10] the boundary condition at the interface between the kinetic
33 and hydrodynamic regions was inferred based on the requirement of the conservation of heat and mass
34 fluxes at this interface. The hydrodynamic heat and mass fluxes were calculated based on the simplifying
35 assumptions that the temperature at the outer boundary of the kinetic region is equal to the droplet surface
36 temperature and vapour pressure at this boundary is equal to the saturated vapour pressure at temperature
37 equal to the droplet surface temperature. The requirement of the conservation of heat and mass fluxes at
38 this interface allowed the authors of the models described in [6]-[8] and [10] to find the corrected values of
39 temperature and vapour density. The main problem with this approach is that the heat and mass fluxes
40 in the hydrodynamic region, calculated based on these corrected values of temperature and vapour density,
41 are not equal to the heat and mass fluxes in the hydrodynamic region used to find these corrected values,

42 in the general case. The only feasible way to overcome this problem seems to be to perform iterations; that
43 is, to use the corrected values of temperature and vapour density (or densities in the case of bi-component
44 droplets) at the outer boundary of the kinetic region to calculate the corrected values of hydrodynamic heat
45 and mass fluxes. The latter in their turn would lead to new corrected values of temperature and vapour
46 density at the outer boundary of the kinetic region etc. If this process converges then we would expect to
47 obtain self-consistent values for both heat and mass fluxes. The main objective of this paper is to present
48 the results of the development of the new kinetic model, based on the above-mentioned iteration process,
49 leading to the discovery of self-consistent heat and mass fluxes, and the application of this model to the
50 analysis of droplet heating and evaporation in realistic Diesel engine-like conditions.

51 The mathematical models, used in the analysis of the processes in the hydrodynamic and kinetic regions,
52 are briefly summarised in Section 2. The iteration processes used in our analysis and the results of their
53 application are described in Section 3 for conditions typical of Diesel engines in the cases where Diesel
54 fuel is approximated by n-dodecane and a mixture of n-dodecane and p-dipropylbenzene. The results of
55 applications of the new model to the analysis of Diesel fuel droplet heating and evaporation in typical Diesel
56 engine-like conditions are presented in Section 4. The main results of the paper are summarised in Section
57 5.

58 2. Mathematical models

59 As in most of our previous papers (e.g. [10]), two regions above the surface of an evaporating fuel
60 droplet, the kinetic and hydrodynamic regions, are considered. We take into account the fact that the
61 thermal conductivity of the liquid phase is finite, and identify the third region as the liquid phase region.
62 All three regions are schematically shown in Fig. 1. T_s and $\rho_s(n,p)$ refer to the surface temperature and vapour
63 density of n-dodecane (n) and p-dipropylbenzene (p) in the immediate vicinity of the droplet surface; T_{Rd} and
64 $\rho_{Rd(n,p)}$ refer to the same parameters but at the interface between the kinetic and the hydrodynamic regions.
65 δ_{Rd} is the thickness of the kinetic region. As in [10], we take into account the diffusion of species in the
66 liquid phase and the presence of up to 3 components in the kinetic region. The conventional hydrodynamic
67 analysis is applied in the liquid and hydrodynamic regions, while vapour and air dynamics in the kinetic
68 region are described by the Boltzmann equations.

69 The mathematical models for all three regions, used in our analysis, are essentially the same as described
70 in [14, 10]. In what follows the most essential features of these models are briefly summarised.

71 As in [14, 10], the effects of finite thermal conductivity and species diffusivity in the liquid phase are
72 taken into account based on the analytical solutions to the heat conduction and species diffusion equations
73 inside droplets, assuming that all processes are spherically symmetric. Both solutions are generalised to the
74 case of moving droplets using the effective thermal conductivity and effective diffusivity models. Raoult's

75 law for the partial pressures of vapour species at the surface of the droplets is assumed to be valid in the
76 case of bi-component droplets. The effects of the curvature of the droplet surface are ignored.

77 A system of up to three Boltzmann equations (for up to two vapour species, and air approximated by
78 nitrogen) is solved in the kinetic region, assuming that the evaporation coefficient for all species is equal to 1.
79 The effects of both elastic and inelastic collisions are taken into account, using the same approach as in [10].
80 The boundary conditions at the interface between the kinetic and hydrodynamic regions are formulated as:

$$\dot{j}_{k(n,p)} = \dot{j}_{h(n,p)} \quad (1)$$

81 (mass flux leaving the kinetic region (k) is equal to the mass flux entering the hydrodynamic region (h) for
82 n-dodecane (n) and p-dipropylbenzene (p)) and

$$q_k = q_h \quad (2)$$

83 (heat flux leaving the kinetic region (k) is equal to the heat flux entering the hydrodynamic region (h)).

84 The values of $\dot{j}_{k(n,p)}$ and q_k were calculated based on the solution to Boltzmann equations, while $\dot{j}_{h(n,p)}$
85 and q_h in the hydrodynamic region were estimated as [14, 10]:

$$\dot{j}_{h(n,p)} = -\frac{\epsilon_i \dot{m}_d}{4\pi R_d^2} = \frac{D_v \rho_{\text{total}}}{2R_d} \epsilon_i \text{Sh}^* \ln(1 + B_M), \quad (3)$$

86 (i refers either to n-dodecane ($i = n$) or p-dipropylbenzene ($i = p$)) and

$$q_h = \frac{k_{\text{mix}}}{R_d} \text{Nu}^* \frac{\ln(1 + B_T)}{2B_T} (T_g - T_{Rd}) = h(T_g - T_{Rd}), \quad (4)$$

87 where

$$\epsilon_i = \frac{Y_{v i R_d}}{\sum_{i=n,p} Y_{v i R_d}}, \quad (5)$$

88 the subscripts v and R_d indicate the vapour phase and the interface between the kinetic and hydrodynamic
89 regions respectively, Y_v is the vapour mass fraction,

$$B_M = \frac{\rho_{v R_d} - \rho_{v \infty}}{\rho_{g R_d}} = \frac{Y_{v R_d} - Y_{v \infty}}{1 - Y_{v R_d}}, \quad (6)$$

90 $B_T = \frac{c_{pv}(T_g - T_s)}{L_{\text{eff}}}$, $L_{\text{eff}} = L + \frac{Q_L}{\dot{m}_d} = \sum_i \epsilon_i L_i + \frac{Q_L}{\sum_i \dot{m}_i}$, Q_L is the power spent on droplet heating, c_{pv} is the
91 specific heat capacity of fuel vapour (estimated for the mixture of vapour species in the case of bi-component
92 droplets), B_T and B_M are linked by the equation

$$B_T = (1 + B_M)^\varphi - 1, \quad (7)$$

$$\varphi = \left(\frac{c_{pv}}{c_{pa}} \right) \left(\frac{\text{Sh}^*}{\text{Nu}^*} \right) \frac{1}{\text{Le}}, \quad (8)$$

Le = $k_a / (c_{pa} \rho_{\text{total}} D_v) = \text{Sc}_d / \text{Pr}_d$ is the Lewis number,

$$\text{Sh}^* = 2 \left(1 + \frac{(1 + \text{Re}_d \text{Sc}_d)^{1/3} \max[1, \text{Re}_d^{0.077}] - 1}{2F(B_M)} \right),$$

$$\text{Nu}^* = 2 \left(1 + \frac{(1 + \text{Re}_d \text{Pr}_d)^{1/3} \max[1, \text{Re}_d^{0.077}] - 1}{2F(B_T)} \right),$$

$$F(B_{T,M}) = (1 + B_{T,M})^{0.7} \frac{\ln(1 + B_{T,M})}{B_{T,M}}, \quad (9)$$

Re_d , Pr_d , Sc_d are Reynolds (based on droplet diameter), Prandtl, and Schmidt numbers respectively, h is the convection heat transfer coefficient. As in the analysis presented in our previous papers (e.g. [10]), we assume that the mass diffusion coefficients in the gas phase for both components (D_v) are the same.

The vapour saturated pressures and other thermodynamic parameters and transport coefficients for liquid and vapour for n-dodecane and p-dipropylbenzene are taken to be the same as in [10] (for n-dodecane these values were ultimately taken from [15]). Thermodynamic and transport properties of the mixture of vapour and air are assumed to be the same as those of pure air (vapour is assumed to be diluted). For example the thermal conductivity of the mixture k_{mix} in Expression (4) is assumed to be equal to that of air. All air properties are taken from [16]. To find the temperature and vapour density at the outer boundary of the kinetic region, Expression (8) was simplified to:

$$\varphi = \left(\frac{c_{pv}}{c_{pa}} \right) \frac{1}{\text{Le}}, \quad (10)$$

assuming that Sh^*/Nu^* is close to 1 (this allowed us to avoid an additional iteration loop on top of the one described in the next section). The general Expression (8) was used in the hydrodynamic calculations, the results of which, in their turn, were used as input parameters in the kinetic model. Equation (10) is strictly valid in the case of stationary droplets only. The validity of this approximation for moving droplets in typical Diesel engine conditions was demonstrated in [17].

All liquid properties are calculated for the average temperature inside droplets. All gas properties are calculated for the reference temperature $T_r = (2/3)T_s + (1/3)T_g$, where T_s and T_g are droplet surface and ambient gas temperature respectively. Enthalpy of evaporation and saturated vapour pressure are estimated at the surface temperature T_s .

Note that the expressions for saturated vapour pressure (p^{sat}) for n-dodecane and p-dipropylbenzene used in our analysis cannot be considered reliable at temperatures close to or above the critical temperatures. Heating and evaporation of the droplets at these temperatures, sometimes predicted by the model at the very final stage of droplet evaporation, does not describe accurately the physical background of the processes at this stage. The contribution of the processes at this stage to the overall droplet heating and evaporation, however, is expected to be small. To mitigate this behaviour of droplet surface temperature, the saturated pressures were artificially increased when the temperatures approached or exceeded the corresponding critical temperatures, using the following formula:

$$p^{\text{sat (corrected)}} = \begin{cases} p^{\text{sat}} & \text{when } T \leq 0.99 T_{\text{cr}} \\ \exp[15(T - 0.99 T_{\text{cr}})/0.99 T_{\text{cr}}] p^{\text{sat}} & \text{when } T > 0.99 T_{\text{cr}}, \end{cases} \quad (11)$$

122 where c_r indicates the critical temperature. This correction affected the very final stage of droplet evaporation
 123 (when their mass becomes less than about 1% of the initial mass in most cases) and produced negligible
 124 effects on the overall process of droplet heating and evaporation.

125 Since the values of fuel vapour density and temperature at level R_d (outer boundary of the kinetic region)
 126 are not known, at the first step these values are assumed equal to those at the droplet surface (level s).

As in [10], the first step in the solution of the Boltzmann equations was to perform an investigation into
 mass and heat transfer processes in the kinetic region for a set of values of ρ_{Rd} (for each of the vapour
 components separately in the case of bi-component droplets) and T_{Rd} . These parameters were assumed to
 be in the ranges: $\rho_{Rd} < \rho_s$ and $T_{Rd} > T_s$ (heating of droplets in a hot gas). For the chosen values of ρ_{Rd} and
 T_{Rd} , the solution to the Boltzmann equations in the kinetic region allowed us to calculate the normalised
 mass and heat fluxes at the outer boundary of this region:

$$\tilde{j}_{k(n,p)} \equiv j_{k(n,p)} / (\rho_0 \sqrt{R_v T_0}), \quad \tilde{q}_k \equiv q_k / (p_0 \sqrt{R_v T_0}),$$

127 where R_v is the gas constant referring to n-dodecane vapour, T_0 is the reference temperature chosen equal
 128 to 600 K, p_0 and ρ_0 are the saturated n-dodecane vapour pressure and density corresponding to T_0 , ρ_0 was
 129 calculated from the ideal gas law. In [8, 10] it was shown that for the case of heating and evaporation of n-
 130 dodecane or a mixture of n-dodecane and p-dipropylbenzene droplets, the values of \tilde{q}_k are almost independent
 131 of $\alpha_\rho \equiv \rho_{Rd} / \rho_s$ in a certain range of α_ρ and the values of \tilde{j}_k are almost independent of $\alpha_T \equiv T_{Rd} / T_s$ in a
 132 certain range of α_T relevant to the conditions typical for Diesel engines.

133 At the same time for both mono- and bi-component droplets it was shown that \tilde{q}_k increases almost
 134 linearly with increasing α_T , and \tilde{j}_k decreases almost linearly with increasing α_ρ . As mentioned earlier, in
 135 our previous papers the values of T_{Rd} and ρ_{Rd} were found from Equations (1) and (2), assuming that $\alpha_T = 1$
 136 and $\alpha_\rho = 1$ for the hydrodynamic model. A more accurate model for finding these parameters, focused on
 137 the calculation of self-consistent fluxes, is described in the next section.

138 3. Calculation of self-consistent mass and heat fluxes

139 Let us assume that Diesel fuel can be approximated by n-dodecane, a droplet is stationary and its
 140 surface temperature is equal to 600 K; gas temperature and pressure are assumed equal to 1000 K and 30
 141 bar respectively. The plots of $\tilde{j}_k \equiv j_{k n} / (\rho_0 \sqrt{R_v T_0})$ versus α_ρ and $\tilde{q}_k \equiv q_k / (p_0 \sqrt{R_v T_0})$ versus α_T are shown
 142 in Figs. 2 and 3 respectively (lines indicated as ‘k’). In the same figures, the plots of $\tilde{j}_h \equiv j_{h n} / (\rho_0 \sqrt{R_v T_0})$
 143 versus α_ρ and $\tilde{q}_h \equiv q_h / (p_0 \sqrt{R_v T_0})$ versus α_T , assuming that $\alpha_\rho = 1$ and $\alpha_T = 1$, are also shown (lines
 144 marked ‘h’, iteration 1). The intersection between these two pairs of lines gave the values $\alpha_\rho = 0.994$ and
 145 $\alpha_T = 1.036$. In our previous analysis these corrections were directly used for calculation of mass and heat
 146 fluxes, taking into account the kinetic effects. In the new model, these corrections are used for updating the

147 values of \tilde{j}_h and \tilde{q}_h , and the updated values of these fluxes are shown in Figs. 2 and 3 as the lines marked ‘h’,
 148 iteration 2. The intersections of these new lines with lines \tilde{j}_k and \tilde{q}_k provide us updated values $\alpha_\rho = 0.993$
 149 and $\alpha_T = 1.034$. Further iterations up to iteration 50 do not lead to any visible changes in these corrections,
 150 as shown in the same Figs. 2 and 3. As follows from the above analysis, the calculation of self-consistent
 151 fluxes leads to a slight decrease in the values of both α_ρ and α_T for a droplet surface temperature of 600 K.
 152 Note that, in contrast to the previously used non-self-consistent model, our new approach does not rely on
 153 the observation that \tilde{q}_k is almost independent of α_ρ and \tilde{j}_k is almost independent of α_T .

154 The same iteration procedure and for the same conditions as presented in Figs. 2 and 3, but for droplets
 155 moving with relative velocity equal to 10 m/s, is shown in Figs. 4 and 5. Comparing the plots shown in Figs.
 156 2 and 3 with those shown in Figs. 4 and 5, one can see that in the case of the moving droplets there is a visible
 157 difference between the values of α_ρ and α_T predicted after the second and 50th iterations. The difference in
 158 the values of α_ρ and α_T inferred from consecutive iterations decreases with increasing iteration number, so
 159 that the differences between these values inferred from the 49th iteration are almost indistinguishable from
 160 those inferred from the 50th iteration. The values of α_ρ and α_T for the self-consistent mass and heat fluxes
 161 predicted for the moving droplet are visibly lower than the ones predicted for the stationary droplet.

162 The same analysis as presented in Figs. 2-5 was repeated for other droplet surface temperatures in the
 163 range 300-650 K and gas temperatures 800 K, 1000 K and 1200 K. Also, the same analysis was repeated for bi-
 164 component droplets (80% n-dodecane and 20% p-dipropylbenzene mixture) for droplet surface temperatures
 165 in the range 300-650 K and gas temperature equal to 1000 K. The predictions of the kinetic model at
 166 temperatures close to the critical temperature of n-dodecane ($T_{cr} = 659$ K) proved to be unreliable and it
 167 was assumed that the values of α_ρ and α_T at $T_s > 650$ K are the same as at $T_s = 650$ K. This assumption
 168 is expected to affect the very final stage of droplet evaporation, and has limited effect on the overall picture
 169 of droplet heating and evaporation. As mentioned in our earlier paper [10], both hydrodynamic and kinetic
 170 models are not reliable at high gas temperature. For example, the derivation of Expression (3) was based on
 171 the assumption that ρ_{total} does not depend on the distance from the droplet surface. This cannot be satisfied
 172 in the case of large differences between the values of droplet surface and gas temperatures. The model in
 173 which this assumption is relaxed was suggested in [18, 19], but it is too complex for use in our analysis, and
 174 is based on several additional assumptions the applicability of which to Diesel engine-like conditions is not
 175 at first evident.

176 The results of the above-mentioned analyses are presented in the form of the plots of α_ρ and α_T versus
 177 droplet surface temperatures T_s for various gas temperatures and droplet velocities and compositions, shown
 178 in Figs. 6-19. Ambient gas pressure in all cases is equal to 30 bar. The plots shown in Figs. 6 and 7 refer
 179 to stationary n-dodecane droplets immersed into gas at temperature 800 K. As can be seen from Fig. 6, the
 180 values of α_ρ decrease with increasing T_s . The values of α_ρ inferred from iteration 2 are slightly lower than
 181 those inferred from iteration 1, and are almost indistinguishable from those inferred from all the following

182 iterations up to iteration 50. The behaviour of the curve α_T versus T_s , shown in Fig. 7, appears to be more
183 complex than that of α_ρ versus T_s . For low temperatures α_T increases with increasing T_s , at intermediate
184 temperatures α_T decreases with increasing T_s , and at temperatures close to 650 K, α_T again increases with
185 increasing T_s . As in the case of α_ρ , the values of α_T inferred from iteration 2 and higher iterations are
186 almost indistinguishable. These values are slightly higher than those inferred from iteration 1 for low T_s
187 and slightly lower than those inferred from iteration 1 for high T_s . In our analysis, the values inferred from
188 iteration 50 are assumed to describe adequately the self-consistent heat and mass fluxes in the vicinity of
189 the surfaces of heated and evaporating droplets.

190 The same plots as presented in Figs. 6 and 7, but for gas temperature equal to 1000 K, are shown in
191 Figs. 8 and 9. The curves shown in Figs. 8 and 9 are similar to those shown in Figs. 6 and 7, except that the
192 difference between the values of α_ρ and α_T inferred from iterations 2-50 and those inferred from iteration
193 1, are larger in the case of gas temperature equal to 1000 K than in the case of gas temperature equal to
194 800 K. The values of these coefficients at $T_s = 600$ K are the same as shown in Figs. 2 and 3.

195 The same plots as presented in Figs. 8 and 9, but for droplets moving with velocity 10 m/s, are shown
196 in Figs. 10 and 11. The general shapes of the curves shown in Figs. 10 and 11 are similar to those shown
197 in Figs. 8 and 9, although comparing these curves one can see that droplet movement leads to increased
198 difference between the values of α_ρ and α_T , inferred from iterations 1 and 2 (and all the following iterations).
199 As can be seen from Fig. 10, the values of α_ρ inferred from iteration 3 are almost indistinguishable from
200 those inferred from iteration 50. This pattern was observed for all other curves although in most cases this
201 is not explicitly demonstrated.

202 The same plots as presented in Figs. 8 and 9, but for gas temperature equal to 1200 K, are shown in
203 Figs. 12 and 13. The curves shown in Figs. 12 and 13 are similar to those shown in Figs. 8 and 9, except
204 that the values of α_ρ tend to be lower and the values of α_T tend to be higher for gas temperature 1200 K
205 compared with the case of gas temperature 1000 K. This shows a tendency for enhanced kinetic effects with
206 increasing gas temperature.

207 Let us now consider the case when Diesel fuel is approximated by a mixture of 80% n-dodecane and
208 20% p-dipropylbenzene and gas temperature and pressure are equal to 1000 K and 30 bar respectively.
209 Droplets are assumed to be stationary. The plots of $\alpha_{\rho n} \equiv \rho_{Rd(n)}/\rho_{s(n)}$ (normalised n-dodecane density)
210 versus T_s , calculated following the procedure shown in Figs. 2 and 4 and inferred from iterations 1-50, are
211 presented in Fig. 14. The results inferred from iteration 2 and all the following iterations turned out to be
212 indistinguishable. Comparing Figs. 14 and 8 one can see that the presence of the second component does
213 not affect the trends of the curves $\alpha_{\rho n}$ versus T_s .

214 The same plots as shown in Fig. 14 but for $\alpha_{\rho p} \equiv \rho_{Rd(p)}/\rho_{s(p)}$ (normalised p-dipropylbenzene density)
215 versus T_s are presented in Fig. 15. Comparing Figs. 15 and 14 one can see that the values of $\alpha_{\rho p}$ are visibly
216 larger than the values of $\alpha_{\rho n}$ (kinetic effects for p-dipropylbenzene are weaker than for n-dodecane).

217 The plots of $\alpha_T \equiv T_{Rd}/T_s$ (normalised temperature at the outer boundary of the kinetic region) versus
 218 T_s , calculated following the procedure shown in Figs. 3 and 5 and inferred from iterations 1-50, are presented
 219 in Fig. 16. The general shapes of the curves shown in this figure are similar to those shown in Figs. 7, 9,
 220 11 and 13. The results for iteration 2 are almost indistinguishable from those for iteration 3 and all the
 221 following iterations up to iteration 50.

222 The same plots as presented in Figs. 14 and 15, but for a droplet moving with velocity 10 m/s, are shown
 223 in Figs. 17 and 18. Comparing the plots shown in Figs. 14 and 15 and those shown in Figs. 17 and 18, one
 224 can see that the movement of droplets leads to increased deviation between the values of coefficients inferred
 225 from iteration 1 and the following iterations.

226 The same plots as presented in Fig. 16, but for the droplet moving with velocity 10 m/s, are shown in
 227 Fig. 19. Comparing the plots shown in Fig. 16 and those shown in Fig. 19, one can see that the movement
 228 of droplets leads to increased deviation between the values of coefficients inferred from iteration 1 and the
 229 following iterations. The values of $\alpha_{\rho n}$ and $\alpha_{\rho p}$ tend to be smaller and the values of α_T tend to be larger
 230 for moving droplets compared with stationary ones.

231 The values of α_ρ ($\alpha_{\rho n}$ and $\alpha_{\rho p}$ in the case of bi-component droplets) and α_T shown in Figs. 6-19 were used
 232 to modify equations for the hydrodynamic model to take into account the kinetic effects. In the case of mono-
 233 component droplets, the corrections α_ρ lead to the replacement of Y_s with $Y_{Rd} = \alpha_\rho Y_s$ and the corresponding
 234 modifications of Spalding numbers B_M and B_T (see Equations (6) and (7)). The modification of B_M leads
 235 to the corresponding modification of the mass flux from the surface of the evaporating droplets (see Equation
 236 (3)). Also, the corrections α_T lead to the replacement of T_s with $T_{Rd} = \alpha_T T_s$. The modifications of B_T and
 237 T_s lead to the modification of the heat flux reaching heated and evaporating droplets described by Equation
 238 (4).

239 In the case of multi-component (bi-component in the case studied in our paper) droplets, the corrections
 240 $\alpha_{\rho n}$ lead to the replacement of $Y_{s(n)}$ with $Y_{Rd(n)} = \alpha_{\rho n} Y_{s(n)}$, and the corrections $\alpha_{\rho p}$ lead to the replace-
 241 ment of $Y_{s(p)}$ with $Y_{Rd(p)} = \alpha_{\rho p} Y_{s(p)}$. The value of Y_{Rd} in this case is calculated as $Y_{Rd(n)} + Y_{Rd(p)}$.
 242 Similarly the value of ϵ_i is modified to take into account the kinetic effects, using the definition of this
 243 parameter (see Equation (5)). The remaining analysis is the same as in the case of the mono-component
 244 droplet.

245 To take into account the kinetic effects in the analytical solution for the temperature inside droplets we
 246 make the following replacement:

$$h \rightarrow h^k = h(B_T^k) \frac{T_g - T_{Rd}}{T_g - T_s} \quad (12)$$

247 In our analysis, the values of α_ρ ($\alpha_{\rho n}$ and $\alpha_{\rho p}$ in the case of bi-component droplets) and α_T shown in
 248 Figs. 6-19 were approximated by analytical formulae shown in Appendix 1. Unfortunately, these analytical
 249 formulae were derived for a limited set of gas temperatures and this limits their potential for implementation

250 in Computational Fluid Dynamics (CFD) codes, to take into account kinetic effects, without first performing
 251 proper kinetic calculations. Once these analytical formulae are obtained for more gas temperatures relevant
 252 to Diesel engine applications, similar analytical expressions describing the effects of gas temperatures on
 253 the values of α_ρ ($\alpha_{\rho n}$ and $\alpha_{\rho p}$ in the case of bi-component droplets) and α_T could potentially be obtained.
 254 This approach could possibly be more efficient for approximating kinetic results compared with the direct
 255 comparison between the values of droplet radii and surface temperatures predicted by hydrodynamic and
 256 kinetic models as suggested in [20]). The feasibility of this approach for a wide range of parameters has yet
 257 to be investigated.

258 In the next section, the results of modelling of Diesel fuel droplet heating and evaporation, using the
 259 model described above, are demonstrated.

260 4. Droplet heating and evaporation

261 The results of calculation of the radii and surface temperatures versus time for a stationary n-dodecane
 262 droplet with initial radius and temperature equal to $5 \mu\text{m}$ and 300 K respectively, immersed into gas with
 263 temperature 1000 K and pressure 30 bar, predicted by the hydrodynamic and kinetic models described in the
 264 previous section (for iteration 50), are shown in Fig. 20. As one can see from this figure, the kinetic effects
 265 lead to a slight reduction of the droplet surface temperature and a noticeable increase in the evaporation
 266 time. This increase is described by parameter E_k , defined as

$$E_k = \frac{t_{e k} - t_{e h}}{t_{e k}} \times 100\%, \quad (13)$$

267 where $t_{e k}$ and $t_{e h}$ are droplet evaporation times predicted by the kinetic and hydrodynamic models respec-
 268 tively. In the case of the plots shown in Fig. 20, $E_k = 3.7\%$.

269 It was shown that the decrease/increase in gas temperature leads to an increase/decrease in the evapo-
 270 ration time as expected. Comparing the calculations for gas temperatures 800 K, 1000 K and 1200 K, and
 271 droplet velocities 0 and 10 m/s we were able to show that for mono-component droplets the relative increase
 272 in the evaporation times due to kinetic effects is more visible at high gas temperatures and droplet velocities.
 273 For stationary droplets the values of E_k increased from 3.2% to 5.0% when gas temperature increased from
 274 800 K to 1200 K. For droplets moving with a velocity of 10 m/s the values of E_k were found to be 5.7%,
 275 6.7% and 6.4% for gas temperatures 800 K, 1000 K and 1200 K, respectively. For all gas temperatures
 276 and droplet velocities under consideration, the kinetic effects led to a slight reduction in the droplet surface
 277 temperature.

278 The same plots as shown in Fig. 20, but for a bi-component droplet (a mixture of 80% n-dodecane and
 279 20% p-dipropylbenzene) are presented in Fig. 21. Comparing the curves shown in Figs. 20 and 21, one can
 280 see that the addition of p-dipropylbenzene leads to a slight increase in the droplet evaporation time, without
 281 noticeable changes in other properties. In this case, $E_k = 2.8\%$.

282 The same plots as shown in Fig. 20, but for a bi-component droplet moving with velocity 10 m/s, are
283 presented in Fig. 22. As in the case of stationary droplets, one can see that the addition of p-dipropylbenzene
284 leads to a slight increase in the droplet evaporation time, without noticeable changes in other properties. In
285 this case, $E_k = 5.7\%$.

286 The plots of mass fractions of n-dodecane ($Y_{s\ n}$) and p-dipropylbenzene ($Y_{s\ p}$) at the surface of the
287 droplet, predicted by hydrodynamic and kinetic models, versus time for the same droplet as described in
288 Fig. 22 are shown in Fig. 23. As one can see from this figure, at the final stage of droplet evaporation the
289 mass fraction of n-dodecane decreases (this is the most volatile component in the mixture) and the mass
290 fraction of p-dipropylbenzene increases (this is the least volatile component in the mixture). This explains
291 why the addition of p-dipropylbenzene leads to an increase in the droplet evaporation time.

292 Note that the analysis so far has been focused on droplets with initial radii $5\ \mu\text{m}$. The kinetic effects
293 decrease with increasing droplet radii (e.g. [20]). For smaller droplet radii, the kinetic effects are expected
294 to be more pronounced compared with those for droplets with radii equal to $5\ \mu\text{m}$. The contribution of
295 these droplets in Diesel engines, however, is expected to be small. Also, the analysis of the kinetic effects
296 for these small droplets would require taking into account the effects of surface tension on the heat transfer
297 and evaporation processes (these were ignored in our analysis).

298 Comparing the plots shown above and the corresponding plots predicted by the non-self-consistent model,
299 described in our previous paper [10], one can see that in most cases the self-consistent model leads to larger
300 kinetic corrections compared with those predicted by the non-self-consistent model for the cases considered
301 in our paper.

302 5. Conclusions

303 A new kinetic model for heating and evaporation of droplets is suggested and applied to the analysis
304 of Diesel fuel droplet heating and evaporation in Diesel engine-like conditions. As in our previous papers
305 (e.g. [8, 10]), the model is based on the introduction of the kinetic region in the immediate vicinity of the
306 heated and evaporating droplets, where the dynamics of molecules are described in terms of the Boltzmann
307 equations for vapour components and air, and the hydrodynamic region. The boundary conditions at the
308 outer boundary of the kinetic region are introduced by matching the heat fluxes and mass fluxes of vapour
309 components leaving the kinetic region and entering into the surrounding hydrodynamic region. The effects
310 of finite thermal conductivity and species diffusivity inside the droplets and inelastic collisions in the kinetic
311 region are taken into account. Diesel fuel is approximated by n-dodecane or a mixture of 80% n-dodecane
312 and 20% p-dipropylbenzene. In both cases, the evaporation coefficient is assumed equal to 1.

313 Attention is drawn to the fact that in the previous papers (e.g. [8, 10]) the heat and mass fluxes in the
314 hydrodynamic region, based on which the temperature and vapour density at the outer boundary of the

315 kinetic region were obtained, were calculated based on the values of temperature and vapour density at the
316 surface of the droplet. These values are not the same as those at the outer boundary of the kinetic region,
317 and this means that the whole approach used in [8, 10] is not self-consistent.

318 To overcome this problem iterations were used. The values of temperature and vapour density at the
319 outer boundary of the kinetic region, obtained following the above-mentioned procedure, were used to
320 calculate the corrected values of hydrodynamic heat and mass fluxes. The latter in their turn led to new
321 corrected values of temperature and vapour density at the outer boundary of the kinetic region etc. It was
322 shown that this process quickly converges for the cases analysed in the paper, and it leads to self-consistent
323 values for both heat and mass fluxes.

324 Following this procedure, a set of coefficients $\alpha_\rho \equiv \rho_{Rd}/\rho_s$ (normalised vapour density at the outer
325 boundary of the kinetic region) and $\alpha_T \equiv T_{Rd}/T_s$ (normalised temperature at the outer boundary of the
326 kinetic region) were obtained for a set of conditions and droplet surface temperatures in the range 300-
327 650 K, assuming that Diesel fuel can be approximated by n-dodecane. In the case when Diesel fuel was
328 approximated by a mixture of n-dodecane and p-dipropylbenzene, α_ρ was replaced with $\alpha_{\rho n} \equiv \rho_{Rd(n)}/\rho_{s(n)}$
329 (normalised n-dodecane density) and $\alpha_{\rho p} \equiv \rho_{Rd(p)}/\rho_{s(p)}$ (normalised p-dipropylbenzene density). These
330 coefficients were implemented into the hydrodynamic code and used for calculation of Diesel fuel droplet
331 heating and evaporation.

332 The model was applied for the analysis of heating and evaporation of Diesel fuel droplets with initial
333 radii and temperature equal to $5 \mu\text{m}$ and 300 K, immersed into gas with temperatures equal to 800 K, 1000
334 K and 1200 K and pressure equal to 30 bar. Droplets were stationary or moving with velocity equal to 10
335 m/s. It was shown that in all cases the kinetic effects led to a decrease in droplet surface temperature and an
336 increase in the evaporation time. This increase is shown to be more visible for higher gas temperatures and
337 moving droplets. The addition of p-dipropylbenzene is shown to decrease the kinetic effects on the droplet
338 evaporation time.

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343

344 References

- 345 [1] S.S. Sazhin, Droplets and Sprays. Springer (2014).
346 [2] N.A. Fuchs, Evaporation and Droplet Growth in Gaseous Media. London: Pergamon Press (1959).

- 347 [3] A.P. Kryukov, V.Yu. Levashov, S.S. Sazhin, Evaporation of Diesel fuel droplets: kinetic versus hydrodynamic models, *Int.*
348 *J. Heat Mass Transfer* 47 (2004) 2541-2549.
- 349 [4] I.N. Shishkova, S.S. Sazhin, A numerical algorithm for kinetic modelling of evaporation processes, *J. Computational*
350 *Physics* 218 (2006) 635-653.
- 351 [5] S.S. Sazhin, I.N. Shishkova, A.P. Kryukov, V.Yu. Levashov, M.R. Heikal, Evaporation of droplets into a background gas:
352 kinetic modelling, *Int. J. Heat Mass Transfer* 50 (2007) 2675-2691.
- 353 [6] S.S. Sazhin, I.N. Shishkova, A kinetic algorithm for modelling the droplet evaporation process in the presence of heat flux
354 and background gas, *Atomization and Sprays* 19 (2009) 473-489.
- 355 [7] I.N. Shishkova, S.S. Sazhin, J.-F. Xie, A solution of the Boltzmann equation in the presence of inelastic collisions, *J.*
356 *Computational Physics* 232 (2013) 87-99.
- 357 [8] S.S. Sazhin, J.-F. Xie, I.N. Shishkova, A.E. Elwardany, M.R. Heikal, A kinetic model of droplet heating and evaporation:
358 effects of inelastic collisions and a non-unity evaporation coefficient, *Int. J. Heat and Mass Transfer* 56 (2013) 525-537.
- 359 [9] I.N. Shishkova, S.S. Sazhin, A solution of the Boltzmann equation in the presence of three components and inelastic
360 collisions, *Int. J. Heat and Mass Transfer* 71 (2014) 26-34.
- 361 [10] S.S. Sazhin, I.N. Shishkova, M. Al Qubeissi, Heating and evaporation of a two-component droplet: Hydrodynamic and
362 kinetic models, *Int. J. Heat and Mass Transfer* 79 (2014) 704-712.
- 363 [11] J.-F. Xie, S.S. Sazhin, B.-Y. Cao, Molecular dynamics study of the processes in the vicinity of the n-dodecane vapour/liquid
364 interface, *Phys. Fluids* 23 (2011) 112104.
- 365 [12] V.M. Gun'ko, R. Nasiri, S.S. Sazhin, Effects of the surroundings and conformerisation of n-dodecane molecules on evapo-
366 ration/condensation processes, *J Chemical Physics* 142 (2015) 034502.
- 367 [13] S.S. Sazhin, V.M. Gun'ko, R. Nasiri, Quantum-chemical analysis of the processes at the surfaces of Diesel fuel droplets,
368 *Fuel* (2016) <http://dx.doi.org/10.1016/j.fuel.2015.10.029> (in press).
- 369 [14] S.S. Sazhin, M. Al Qubeissi, R. Nasiri, V.M. Gunko, A.E. Elwardany, F. Lemoine, F., Grisch, M.R. Heikal, A multi-
370 dimensional quasi-discrete model for the analysis of Diesel fuel droplet heating and evaporation, *Fuel* 129 (2004) 238-266.
- 371 [15] B. Abramzon, S.S. Sazhin, Convective vaporization of fuel droplets with thermal radiation absorption, *Fuel* 85 (2006)
372 32-46.
- 373 [16] F.P. Incropera, D.P. DeWitt, *Fundamentals of Heat and Mass Transfer*, Fifth Edition. New York, Chichester: John Wiley
374 & Sons (2002).
- 375 [17] A.E. Elwardany, I.G. Gusev, G. Castanet, F. Lemoine, S.S. Sazhin, Mono- and multi-component droplet cooling/heating
376 and evaporation: comparative analysis of numerical models, *Atomization and Sprays* 21 (2011), 907-931.
- 377 [18] S. Tonini, G.E. Cossali, An analytical model of liquid drop evaporation in gaseous environment. *Int. J. Thermal Sciences*
378 57 (2012) 45-53.
- 379 [19] S. Tonini, G.E. Cossali, A novel vaporisation model for a single-component drop in high temperature air streams. *Int. J.*
380 *Thermal Sciences* 75 (2014) 194-203.
- 381 [20] S.S. Sazhin, I.N. Shishkova, M. Heikal, Kinetic modelling of fuel droplet heating and evaporation: calculations and
382 approximations, *Int. J. Engineering Systems Modelling and Simulation* 2 (2010), 169-176.

383 Figure Captions

384

385 **Fig. 1** Liquid, kinetic and hydrodynamic regions near the surface of the droplet. T_s is the droplet surface
386 temperature, $\rho_s(n,p)$ are n-dodecane (n) and p-dipropylbenzene (p) vapour densities in the immediate vicin-

387 ity of the droplet surface, T_{Rd} and $\rho_{Rd(n,p)}$ are the temperature and n-dodecane (n) and p-dipropylbenzene
388 (p) vapour densities at the outer boundary of the kinetic region.

389
390 **Fig. 2** The plots of normalised mass fluxes $\tilde{j} \equiv j/(\rho_0\sqrt{R_vT_0})$ predicted by the kinetic (line 'k') and hy-
391 drodynamic (lines 'h') models for a stationary n-dodecane droplet versus $\alpha_\rho \equiv \rho_{Rd}/\rho_s$ (normalised vapour
392 density at the outer boundary of the kinetic region). Droplet surface and gas temperatures are assumed
393 equal to 600 K and 1000 K respectively. The values of α_ρ inferred from iteration 2 and higher iterations are
394 indistinguishable.

395
396 **Fig. 3** The plots of normalised heat fluxes $\tilde{q} \equiv q/(\rho_0\sqrt{R_vT_0})$ predicted by the kinetic (line 'k') and
397 hydrodynamic (lines 'h') models for a stationary n-dodecane droplet versus $\alpha_T \equiv T_{Rd}/T_s$ (normalised tem-
398 perature at the outer boundary of the kinetic region). Droplet surface and gas temperatures are assumed
399 equal to 600 K and 1000 K respectively. The values of α_T inferred from iteration 2 and higher iterations
400 are indistinguishable.

401
402 **Fig. 4** The same as Fig. 2 but for a droplet moving with velocity 10 m/s. In this case there is a visible
403 difference between the results inferred from iteration 2 and iteration 50.

404
405 **Fig. 5** The same as Fig. 3 but for a droplet moving with velocity 10 m/s. In this case there is a visible
406 difference between the results inferred from iteration 2 and iteration 50.

407
408 **Fig. 6** The plots of α_ρ versus T_s for a stationary n-dodecane droplet immersed in gas (air) at temperature
409 equal to 800 K. The values of α_ρ inferred from iteration 2 and higher iterations are indistinguishable.

410
411 **Fig. 7** The plots of α_T versus T_s for a stationary n-dodecane droplet immersed in gas (air) at tempera-
412 ture equal to 800 K. The values of α_T inferred from iteration 2 and higher iterations are indistinguishable.

413
414 **Fig. 8** The plots of α_ρ versus T_s for a stationary n-dodecane droplet immersed in gas (air) at temperature
415 equal to 1000 K. The values of α_ρ inferred from iteration 2 and higher iterations are indistinguishable.

416
417 **Fig. 9** The plots of α_T versus T_s for a stationary n-dodecane droplet immersed in gas (air) at tempera-
418 ture equal to 1000 K. The values of α_T inferred from iteration 2 and higher iterations are indistinguishable.

419
420 **Fig. 10**
421 The plots of α_ρ versus T_s for a n-dodecane droplet moving with velocity 10 m/s in gas (air) at temper-

422 ature equal to 1000 K.

423

424 **Fig. 11** The plots of α_T versus T_s for a n-dodecane droplet moving with velocity 10 m/s in gas (air) at
425 temperature equal to 1000 K.

426

427 **Fig. 12** The plots of α_ρ versus T_s for a stationary n-dodecane droplet immersed in gas (air) at tempera-
428 ture equal to 1200 K. The values of α_ρ inferred from iteration 2 and higher iterations are indistinguishable.

429

430 **Fig. 13** The plots of α_T versus T_s for a stationary n-dodecane droplet immersed in gas (air) at tempera-
431 ture equal to 1200 K. The values of α_T inferred from iteration 2 and higher iterations are indistinguishable.

432

433 **Fig. 14** The plots of $\alpha_{\rho n} \equiv \rho_{Rd(n)}/\rho_{s(n)}$ (normalised n-dodecane density) versus T_s for a stationary
434 bi-component droplet (a mixture of 80% n-dodecane and 20% p-dipropylbenzene) immersed in gas (air) at
435 temperature equal to 1000 K. The values of α_ρ inferred from iteration 2 and higher iterations are indistin-
436 guishable.

437

438 **Fig. 15** The plots of $\alpha_{\rho p} \equiv \rho_{Rd(p)}/\rho_{s(p)}$ (normalised p-dipropylbenzene density) versus T_s for a sta-
439 tionary bi-component droplet (a mixture of 80% n-dodecane and 20% p-dipropylbenzene) immersed in gas
440 (air) at temperature equal to 1000 K. The values of α_ρ inferred from iteration 2 and higher iterations are
441 indistinguishable.

442

443 **Fig. 16** The plots of α_T versus T_s for a stationary bi-component droplet (a mixture of 80% n-dodecane
444 and 20% p-dipropylbenzene) immersed in gas (air) at temperature equal to 1000 K. The values of α_ρ inferred
445 from iteration 2 and higher iterations are indistinguishable.

446

447 **Fig. 17** The plots of $\alpha_{\rho n} \equiv \rho_{Rd(n)}/\rho_{s(n)}$ (normalised n-dodecane density) versus T_s for a bi-component
448 droplet (a mixture of 80% n-dodecane and 20% p-dipropylbenzene) moving with velocity 10 m/s in gas (air)
449 at temperature equal to 1000 K.

450

451 **Fig. 18** The plots of $\alpha_{\rho p} \equiv \rho_{Rd(p)}/\rho_{s(p)}$ (normalised p-dipropylbenzene density) versus T_s for a bi-
452 component droplet (a mixture of 80% n-dodecane and 20% p-dipropylbenzene) moving with velocity 10 m/s
453 in gas (air) at temperature equal to 1000 K.

454

455 **Fig. 19** The plots of α_T versus T_s for a bi-component droplet (a mixture of 80% n-dodecane and 20%
456 p-dipropylbenzene) moving with velocity 10 m/s in gas (air) at temperature equal to 1000 K.

457

458 **Fig. 20** The plots of R_d and T_s versus time, as predicted by the kinetic (solid) and hydrodynamic
459 (dashed) models for a stationary n-dodecane droplet with initial radius and temperature equal to $5\ \mu\text{m}$ and
460 300 K, respectively, immersed in a gas (air) at temperature 1000 K.

461

462 **Fig. 21** The same as Fig. 20, but for a stationary bi-component droplet (a mixture of 80% n-dodecane
463 and 20% p-dipropylbenzene).

464

465 **Fig. 22** The same as Fig. 21, but for a droplet moving with velocity 10 m/s.

466

467 **Fig. 23** The same as Fig. 22, but for mass fractions of n-dodecane (Y_n) and p-dipropylbenzene (Y_p) at
468 the surface of the droplet.

469

470

471 **Appendix 1**

472 **Approximations of α_ρ , $\alpha_{\rho n}$, $\alpha_{\rho p}$ and α_T versus T_s (iteration 50)**

473 All approximations have been obtained for temperatures T_s in the range 300-650 K.

474

Figs. (6) and (7) ($T_g = 800$ K, a stationary n-dodecane droplet):

$$\begin{aligned}\alpha_\rho &= 0.95127 + 6.62107 \cdot 10^{-4} T_s - 3.55461 \cdot 10^{-6} T_s^2 + 9.36931 \cdot 10^{-9} T_s^3 - 1.2005 \cdot 10^{-11} T_s^4 \\ &\quad + 5.87685 \cdot 10^{-15} T_s^5, \\ \alpha_T &= 2.16074 - 0.01843 T_s + 1.24389 \cdot 10^{-4} T_s^2 - 4.59688 \cdot 10^{-7} T_s^3 + 1.00627 \cdot 10^{-9} T_s^4 \\ &\quad - 1.30565 \cdot 10^{-12} T_s^5 + 9.29602 \cdot 10^{-16} T_s^6 - 2.80028 \cdot 10^{-19} T_s^7.\end{aligned}$$

475

Figs. (8) and (9) ($T_g = 1000$ K, a stationary n-dodecane droplet):

$$\begin{aligned}\alpha_\rho &= 0.97924 + 3.38661 \cdot 10^{-4} T_s - 2.10013 \cdot 10^{-6} T_s^2 + 6.19675 \cdot 10^{-9} T_s^3 - 0.864558 \cdot 10^{-11} T_s^4 \\ &\quad + 4.47852 \cdot 10^{-15} T_s^5, \\ \alpha_T &= 3.09685 - 0.03312 T_s + 2.22137 \cdot 10^{-4} T_s^2 - 8.15444 \cdot 10^{-7} T_s^3 + 1.77164 \cdot 10^{-9} T_s^4 \\ &\quad - 2.27837 \cdot 10^{-12} T_s^5 + 16.049 \cdot 10^{-16} T_s^6 - 4.77199 \cdot 10^{-19} T_s^7.\end{aligned}$$

476

Figs. (10) and (11) ($T_g = 1000$ K, an n-dodecane droplet moving with relative velocity 10 m/s):

$$\begin{aligned}\alpha_\rho &= 1.37063 - 0.00428 T_s + 1.88185 \cdot 10^{-5} T_s^2 - 3.89817 \cdot 10^{-8} T_s^3 + 3.7469 \cdot 10^{-11} T_s^4 \\ &\quad - 1.34491 \cdot 10^{-14} T_s^5, \\ \alpha_T &= 4.74618 - 0.05942 T_s + 4.02544 \cdot 10^{-4} T_s^2 - 1.49552 \cdot 10^{-6} T_s^3 + 3.2968 \cdot 10^{-9} T_s^4 \\ &\quad - 4.31537 \cdot 10^{-12} T_s^5 + 3.1035 \cdot 10^{-15} T_s^6 - 9.44769 \cdot 10^{-19} T_s^7.\end{aligned}$$

477

Figs. (12) and (13) ($T_g = 1200$ K, a stationary n-dodecane droplet):

$$\begin{aligned}\alpha_\rho &= 1.02633 - 2.13871 \cdot 10^{-4} T_s + 4.31389 \cdot 10^{-7} T_s^2 + 5.43478 \cdot 10^{-10} T_s^3 - 2.48699 \cdot 10^{-12} T_s^4 \\ &\quad + 1.84009 \cdot 10^{-15} T_s^5, \\ \alpha_T &= 3.60953 - 0.04105 T_s + 2.74138 \cdot 10^{-4} T_s^2 - 1.00118 \cdot 10^{-6} T_s^3 + 2.16179 \cdot 10^{-9} T_s^4\end{aligned}$$

$$-2.75897 \cdot 10^{-12} T_s^5 + 1.92458 \cdot 10^{-15} T_s^6 - 5.65003 \cdot 10^{-19} T_s^7.$$

478

Figs. (14), (15) and (16) ($T_g = 1000$ K, a stationary bi-component (a mixture of 80% n-dodecane and 20% p-dipropylbenzene) droplet):

$$\begin{aligned} \alpha_{\rho n} &= 0.84400 + 0.00193 T_s - 9.46424 \cdot 10^{-6} T_s^2 + 2.29404 \cdot 10^{-8} T_s^3 - 2.736 \cdot 10^{-11} T_s^4 \\ &\quad + 1.27255 \cdot 10^{-14} T_s^5, \\ \alpha_{\rho p} &= 0.95587 + 5.37126 \cdot 10^{-4} T_s - 2.58165 \cdot 10^{-6} T_s^2 + 6.11316 \cdot 10^{-9} T_s^3 - 7.10412 \cdot 10^{-12} T_s^4 \\ &\quad + 3.21354 \cdot 10^{-15} T_s^5, \\ \alpha_T &= 2.62683 - 0.0219 T_s + 1.21723 \cdot 10^{-4} T_s^2 - 3.55272 \cdot 10^{-7} T_s^3 + 5.75889 \cdot 10^{-10} T_s^4 \\ &\quad - 4.92827 \cdot 10^{-13} T_s^5 + 1.74267 \cdot 10^{-16} T_s^6. \end{aligned}$$

479

Figs. (17), (18) and (19) ($T_g = 1000$ K, a bi-component (a mixture of 80% n-dodecane and 20% p-dipropylbenzene) droplet moving with relative velocity 10 m/s):

$$\begin{aligned} \alpha_{\rho n} &= 0.96092 + 6.31887 \cdot 10^{-4} T_s - 4.26513 \cdot 10^{-6} T_s^2 + 1.42574 \cdot 10^{-8} T_s^3 - 2.27105 \cdot 10^{-11} T_s^4 \\ &\quad + 1.3282 \cdot 10^{-14} T_s^5, \\ \alpha_{\rho p} &= 0.93763 + 7.74252 \cdot 10^{-4} T_s - 3.86981 \cdot 10^{-6} T_s^2 + 9.71485 \cdot 10^{-9} T_s^3 - 1.21398 \cdot 10^{-11} T_s^4 \\ &\quad + 5.90554 \cdot 10^{-15} T_s^5, \\ \alpha_T &= 5.8157 - 0.06441 T_s + 3.55615 \cdot 10^{-4} T_s^2 - 1.02948 \cdot 10^{-6} T_s^3 + 1.65178 \cdot 10^{-9} T_s^4 \\ &\quad - 1.39642 \cdot 10^{-12} T_s^5 + 4.86933 \cdot 10^{-16} T_s^6. \end{aligned}$$

480

481 The accuracy of these approximations for α_{ρ} and α_T for stationary n-dodecane droplets immersed in gas
482 (air) at temperature 1000 K is illustrated in Figs. A1 and A2. The accuracy of the same approximations
483 but for a droplet moving with relative velocity 10 m/s is illustrated in Figs. A3 and A4.

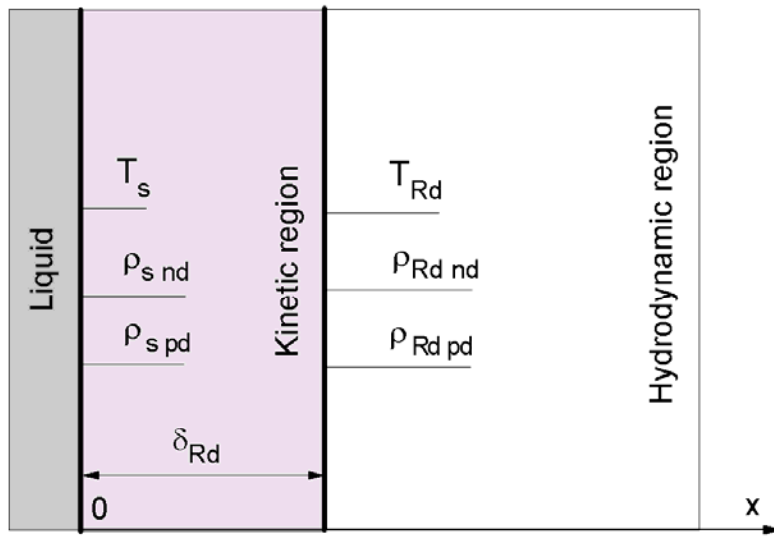


Fig.1.

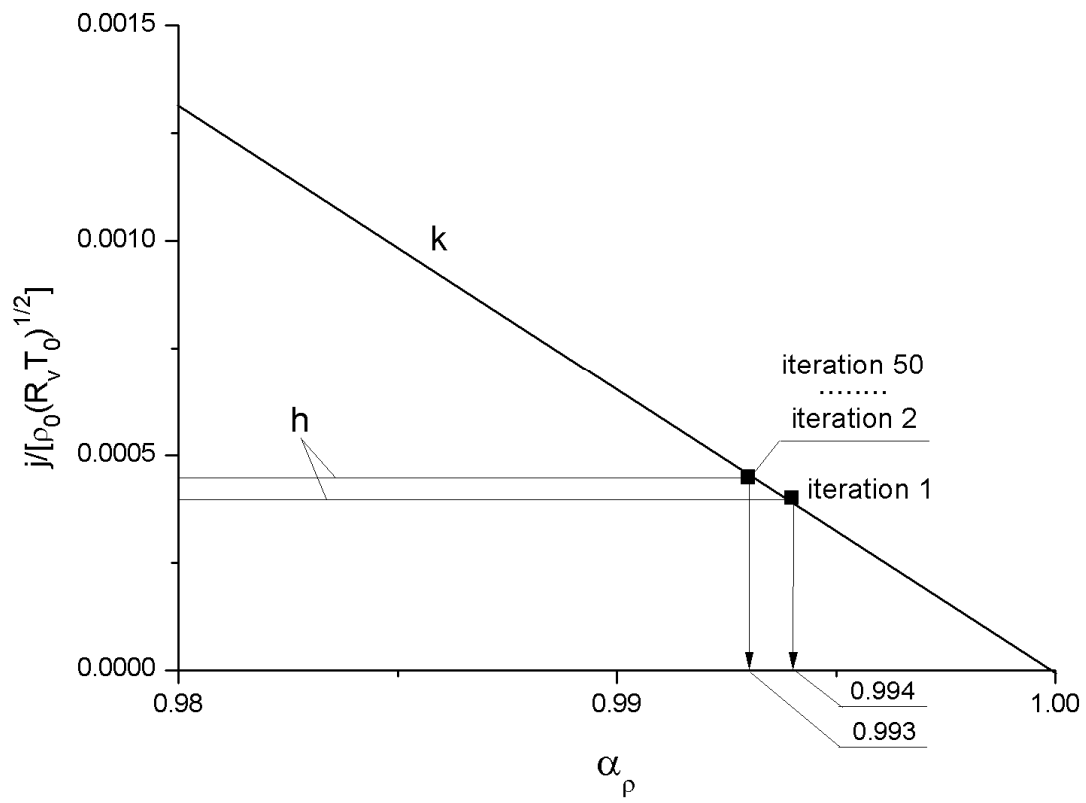


Fig.2.

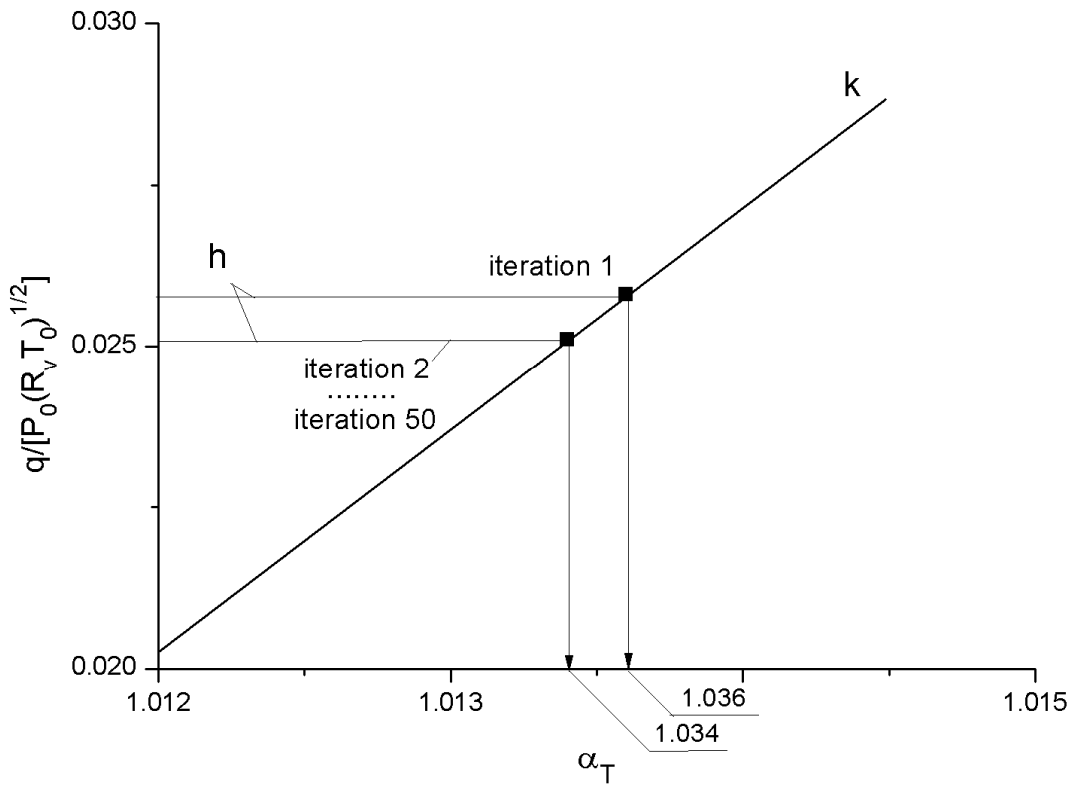


Fig.3.

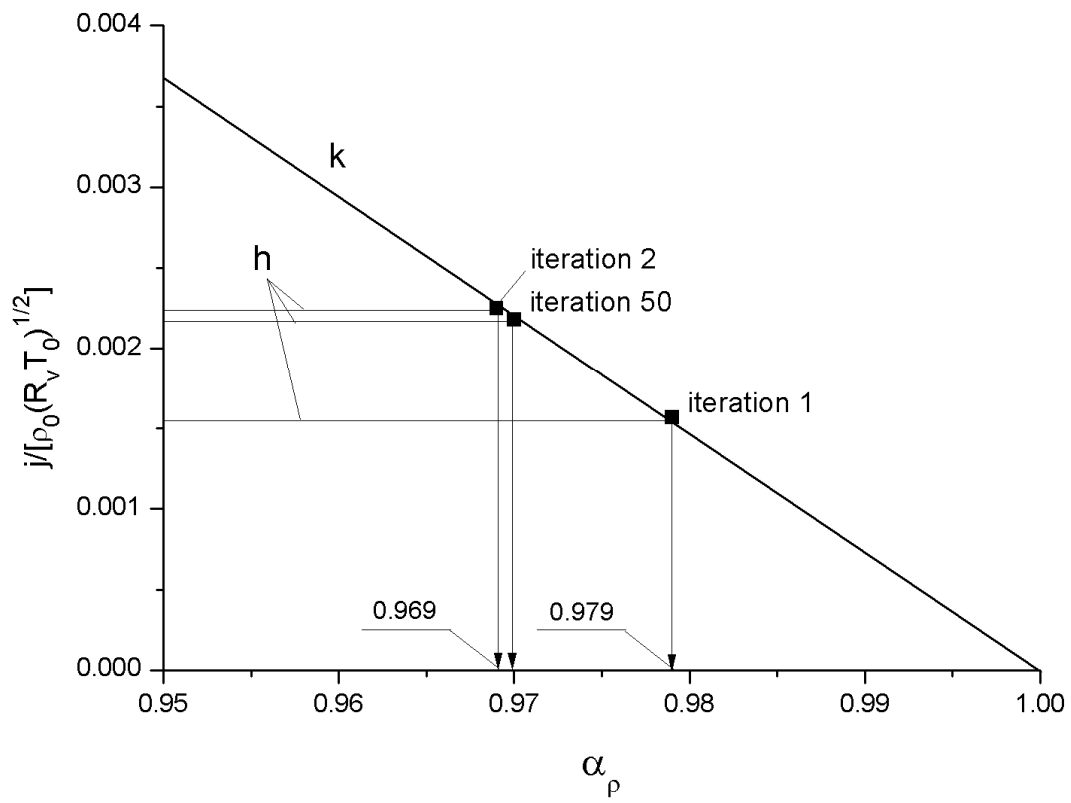


Fig.4.

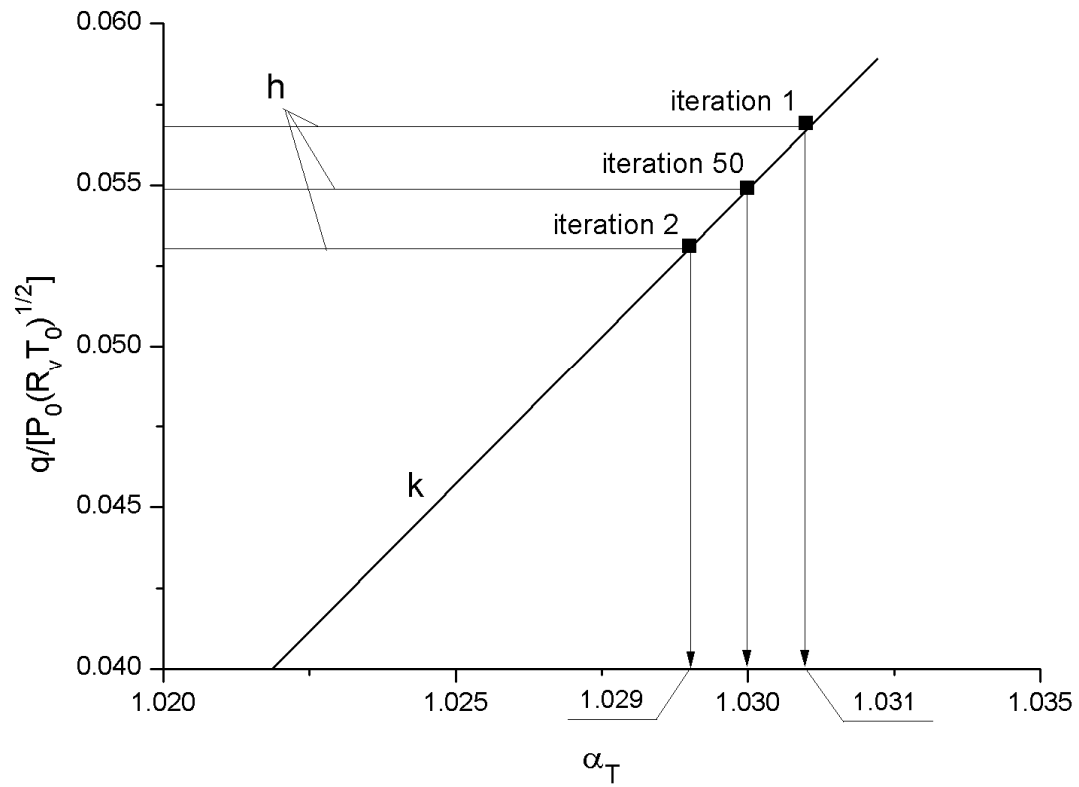


Fig.5.

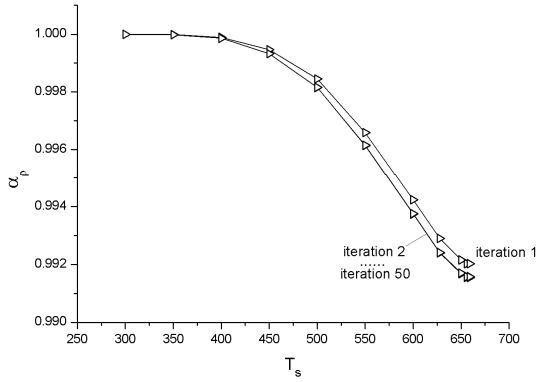


Fig.6.

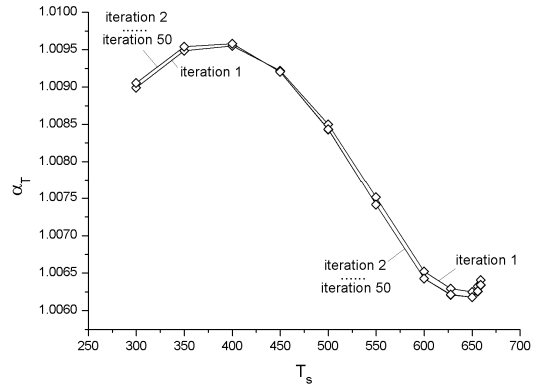


Fig.7.

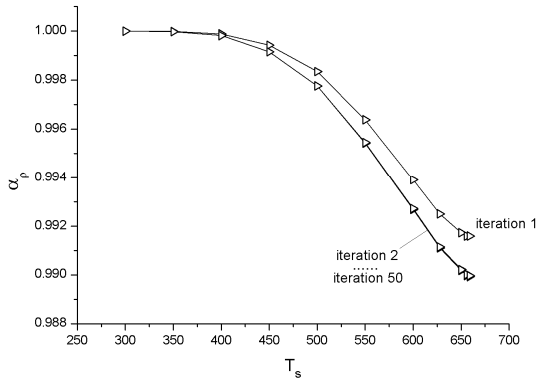


Fig.8.

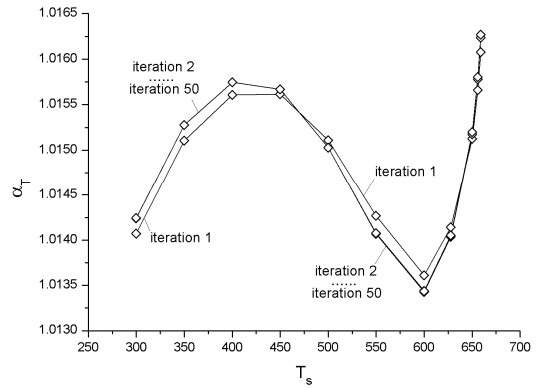


Fig.9.

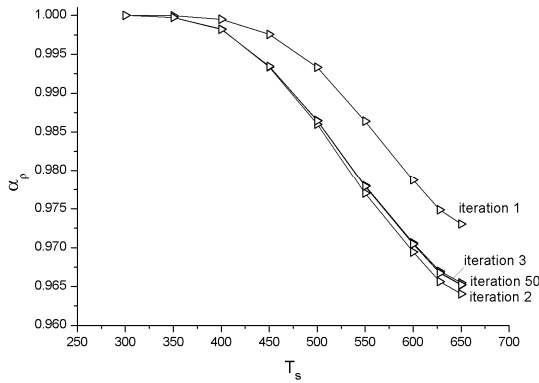


Fig.10.

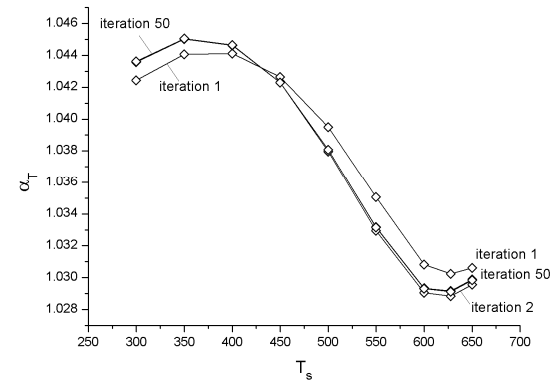


Fig.11.

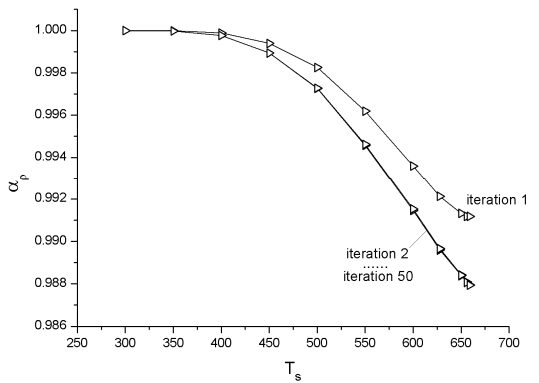


Fig.12.

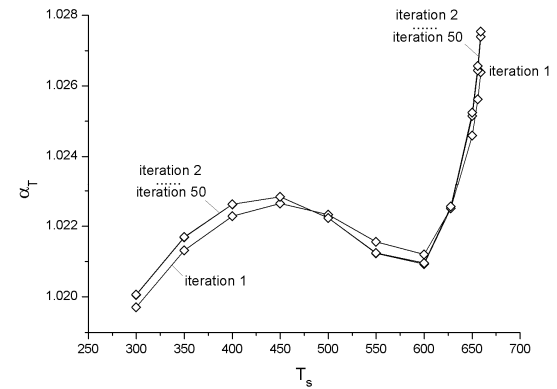


Fig.13.

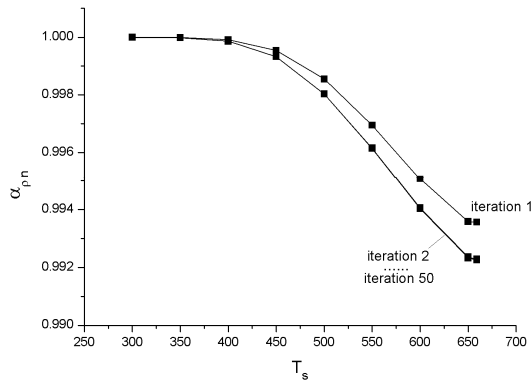


Fig.14.

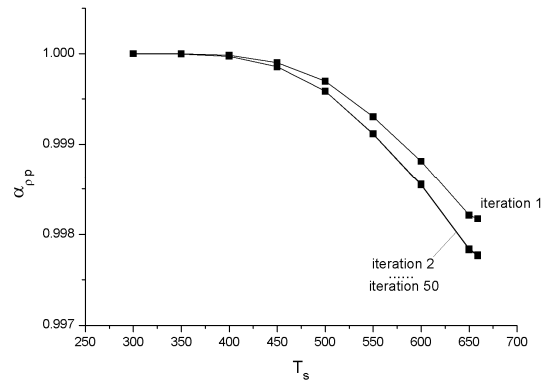


Fig.15.

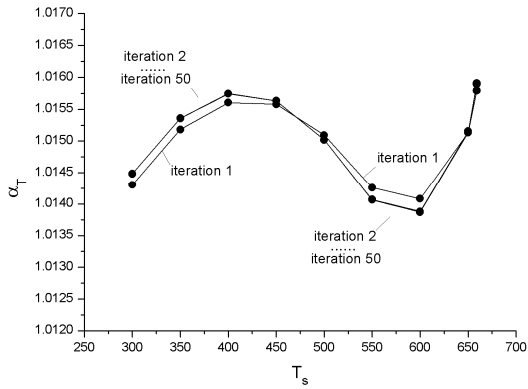


Fig.16.

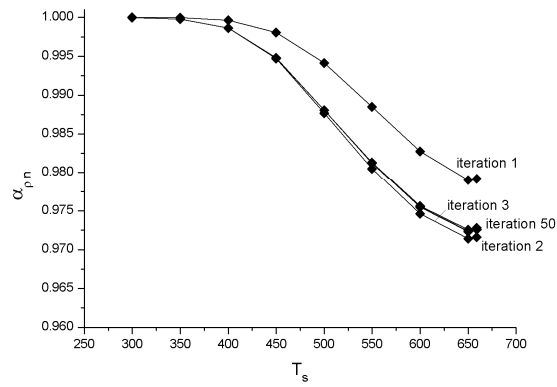


Fig.17.

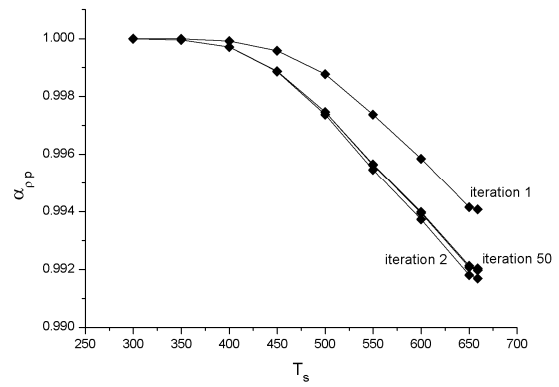


Fig.18.

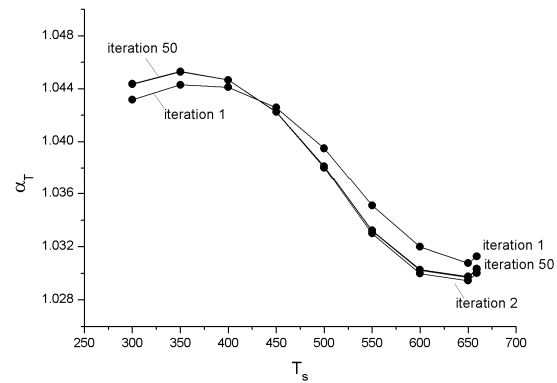


Fig.19.

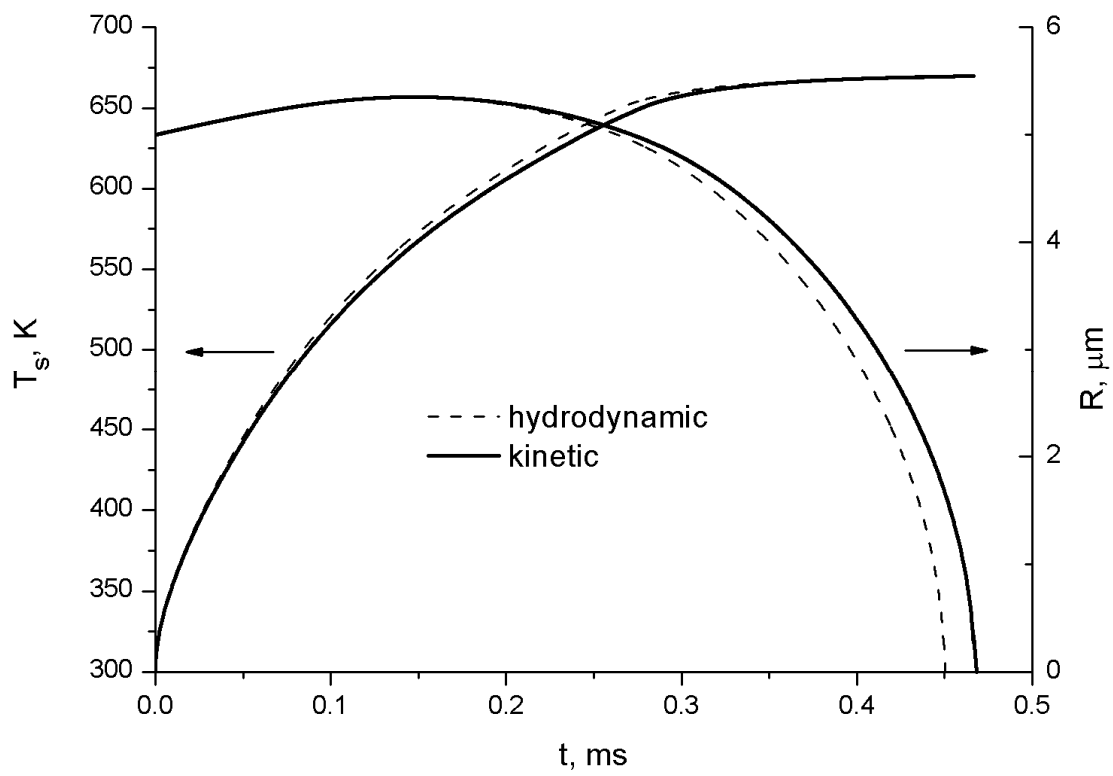


Fig.20.

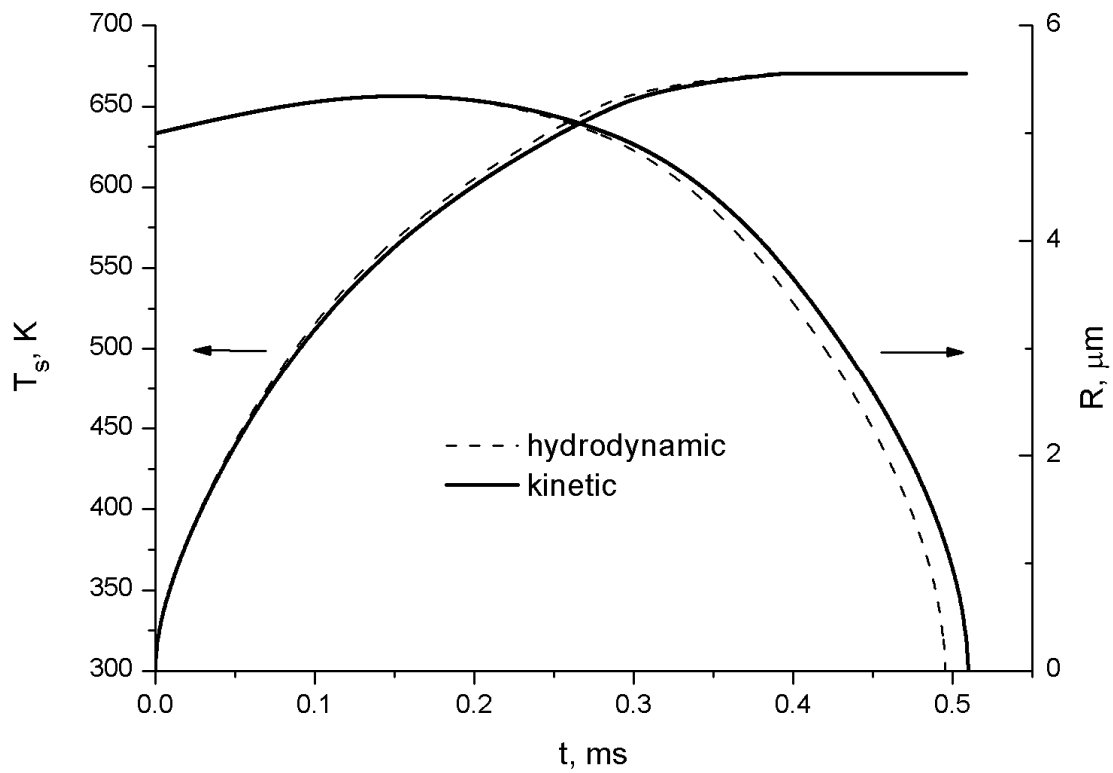


Fig.21.

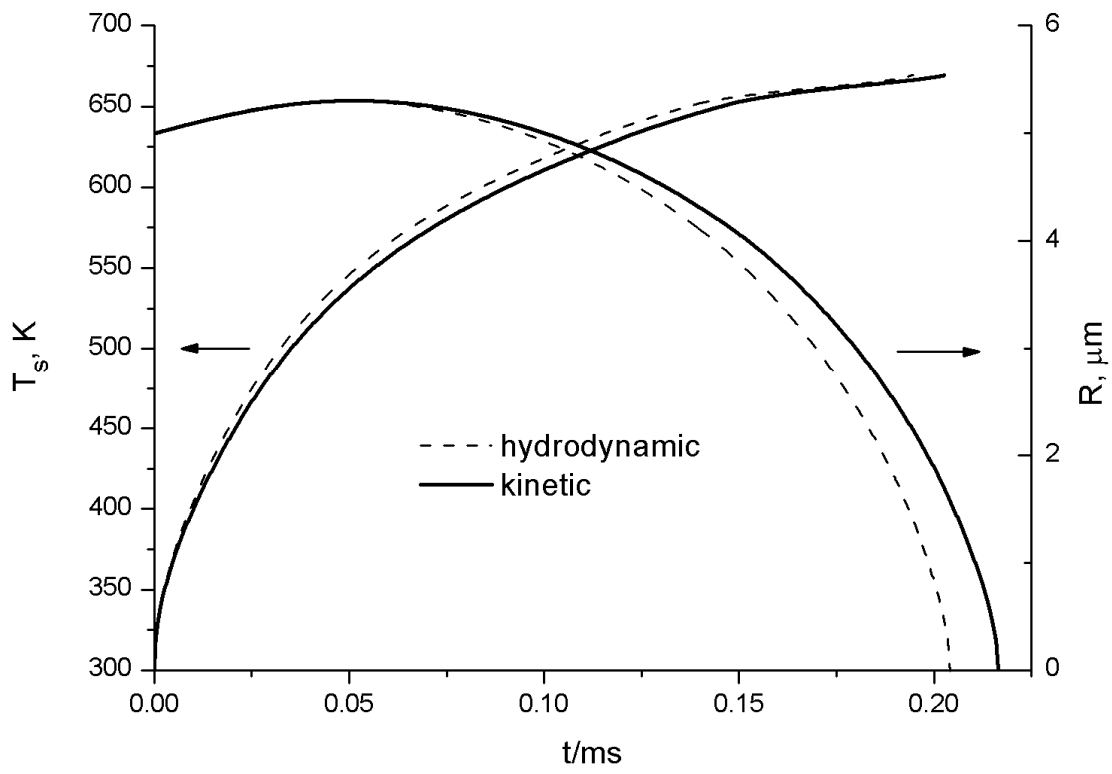


Fig.22.

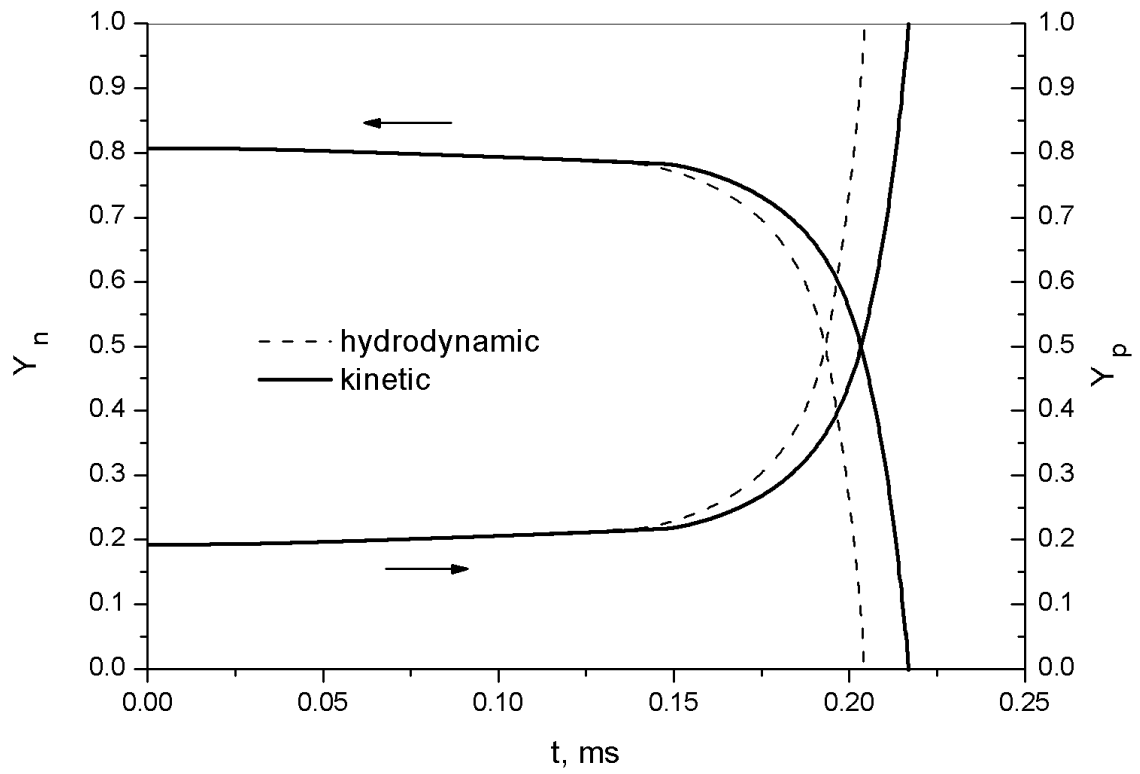


Fig.23.

Appendix

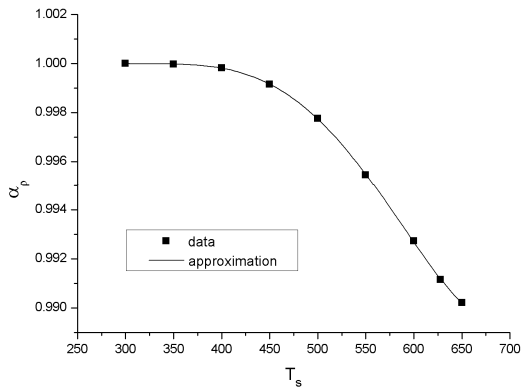


Fig.A1.

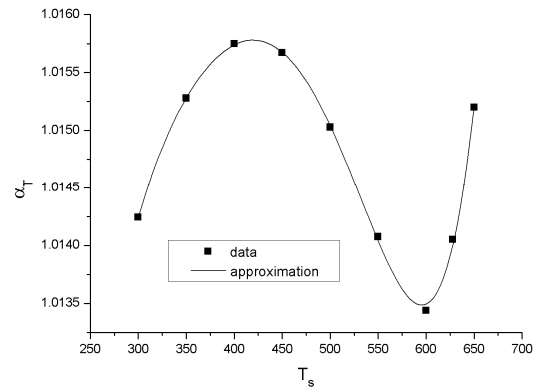


Fig.A2.

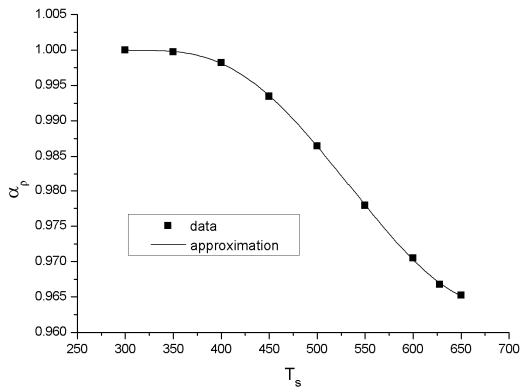


Fig.A3.

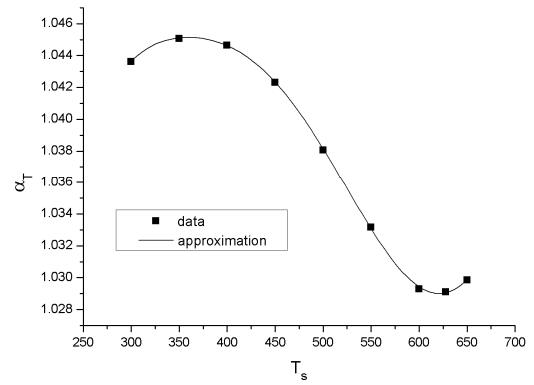


Fig.A4.