A model for multi-component droplet heating and evaporation and its implementation into ANSYS Fluent

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Abstract

The main ideas of the model for multi-component droplet heating and evaporation, based on the analytical solutions to the heat conduction and species diffusion equations in the liquid phase, and its implementation into ANSYS Fluent CFD software are described. The model is implemented into this software via User-Defined Functions (UDF). The predictions of ANSYS Fluent with the newly implemented model are verified against the results predicted by the previously developed in-house research code for droplets comprising of a mixture of ethanol and acetone evaporating and cooled down in ambient air.

Key words: Droplets, heating, evaporation, ANSYS Fluent, ethanol, acetone

Nomenclature

d	diameter of a droplet
D	diffusion coefficient
h_{Y0}	parameter defined by Equation (2)

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$\dot{m}$	evaporation rate
N_{L}	number of layers inside a droplet
Pe	Peclet number
Pr	Prandtl number
q_{Yin}	parameter defined by Equation (4)
Q_{Yn}	parameter defined by Equation (3)
R	radial coordinate from the centre of the droplet
R_{d}	radius of a droplet
Re	Reynolds number
Sc	Schmidt number
t	time
T	temperature
v	velocity
v_{Yn}	eigenfunction
Y	mass fraction

Greek symbols

α_m	parameter defined by (7)
ε_i	parameter defined by (8)
λ_n	eigenvalues
ν	kinematic viscosity
ρ	density
χ_Y	correction function defined by Equation (10)

Subscripts

a	acetone
d	droplet
eff	effective
e	ethanol
g	gas
i	species
l	liquid phase
ref	reference value
s	surface of droplet
v	vapour phase
0	value at the beginning of a time step

1. Introduction

A model for mono- and multi-component droplet heating and evaporation, based on the analytical solutions to the heat transfer and species diffusion equations, is described in [1, 2]. This model has been validated based on available experimental data and verified based on the predictions of the numerical code using the numerical solutions to these equations [3, 4]. Although the importance and efficiency of this approach to the modelling of these processes have been clearly demonstrated [1, 2], the applicability of this model to the analysis of realistic engineering processes, including those which take place in internal combustion engines [5], turned out to be limited. The main reason for this limitation is that in most realistic engineering applications, heating and evaporation of droplets take place not in isolation but in close interaction with a number of other processes, including hydrodynamic and heat/mass transfer processes in the carrier phase and chemical reactions. The interactions between these processes are taken into account in numerous research and commercial CFD codes.

The authors of [6] were perhaps the first to describe the preliminary results of implementation of a model for droplet heating and evaporation, taking into account the effects of temperature gradient and recirculation inside an individual droplet, into the commercial CFD software ANSYS Fluent. This problem was investigated later in more detail in [7]. In the latter paper, the results of the implementation of the model of mono-component droplet heating and evaporation into ANSYS Fluent, using User-Defined Functions (UDF), was described. The predictions of the customised version of ANSYS Fluent were compared with the results of experimental measurements performed at the Combustion Research Facility, Sandia National Laboratories, and verified using the results predicted by in-house research code for an n-dodecane droplet heated and evaporated in hot air [7]. The main limitation of the model described in [7] is that it is applicable only to mono-component droplets, while most droplets used in engineering, including automotive, applications are multi-component. For the case of multi-component droplets, the process of species diffusion inside them needs to be taken into account alongside the heat transfer process [1, 2]. The characteristic times of species diffusion are generally much longer than temperature relaxation times. Thus, taking into account species diffusion inside droplets is expected to be even more important than taking into account temperature gradients.

The main focus of this paper is on the generalisation of the results re-

ported in [7], to the case of multi-component droplets, using the results of preliminary analysis presented in [6]. The model to be used in our analysis is based on the analytical solutions to the heat transfer and species diffusion equations in the liquid phase and is described in detail in [1, 2]. The effect of recirculation in the liquid phase is taken into account based on the Effective Thermal Conductivity (ETC)/ Effective Diffusivity (ED) model [1, 2]. The Abramzon and Sirignano approach [8] is used for modelling of the gas phase.

The main ideas of the model for temperature distribution in the droplets, used in our analysis, are summarised in [7] and will not be repeated in this paper. The model for species diffusion in the droplets, based on the analytical solution to the species diffusion equation, is briefly summarised in Section 2. Then the details of the implementation of the model into ANSYS Fluent are described (Section 3). The predictions of the version of ANSYS Fluent, with the new model implemented into it, are then compared with the predictions of the previously developed one-dimensional in-house code for the case of heating/cooling and evaporation of acetone/ethanol droplets (Section 4). The choice of these droplets was based on the fact that the predictions of the one-dimensional in-house code for them were validated against experimental data and verified against the predictions of the numerical code using the numerical solutions to these equations [3, 4]. Then the main results of the paper are summarised.

2. Basic equations

As in the case of the heat transfer equation inside droplets, we assume that species diffusion inside them is described by the one-dimensional species diffusion equation and all processes are spherically symmetric. Assuming that droplet radius $R_{\rm d}$ is constant (an approximation valid for short time steps), the analytical solution to this equation for the mass fractions $Y_{{\rm l},i}$, subject to the initial condition $Y_{{\rm l},i}(t=0,R)=Y_{{\rm l},i0}(R)$, is presented as [1]:

$$Y_{{\rm l},i}=\varepsilon_i+\frac{1}{R}\left\{\exp\left[D_{\rm l}\left(\frac{\lambda_0}{R_{\rm d}}\right)^2 t\right]\left[q_{Yi0}-Q_{Y0}\epsilon_i\right]\sinh\left(\lambda_0\frac{R}{R_{\rm d}}\right)\right.$$

$$\left.+\sum_{n=1}^{\infty}\left[\exp\left[-D_{\rm l}\left(\frac{\lambda_n}{R_{\rm d}}\right)^2 t\right]\left[q_{Yin}-Q_{Yn}\epsilon_i\right]\sin\left(\lambda_n\frac{R}{R_{\rm d}}\right)\right]\right\}, \qquad (1)$$

where λ_0 and λ_n ($n \geq 1$) are solutions to the equations

$$\tanh\lambda = -\frac{\lambda}{h_{Y0}} \qquad \text{and} \qquad \tan\lambda = -\frac{\lambda}{h_{Y0}},$$

respectively,

$$h_{Y0} = -\left(1 + \frac{\alpha_m R_\mathrm{d}}{D_\mathrm{l}}\right), \tag{2}$$

$$Q_{Yn} = \begin{cases} -\frac{1}{||v_{Y0}||^2}\left(\frac{R_\mathrm{d}}{\lambda_0}\right)^2 (1+h_{Y0})\sinh\lambda_0 & \text{when} \quad n=0 \\ \frac{1}{||v_{Yn}||^2}\left(\frac{R_\mathrm{d}}{\lambda_n}\right)^2 (1+h_{Y0})\sin\lambda_n & \text{when} \quad n\geq 1 \end{cases} \tag{3}$$

$$q_{Yin} = \frac{1}{||v_{Yn}||^2}\int_0^{R_\mathrm{d}} R Y_{\mathrm{li}0}(R) v_{Yn}(R)\mathrm{d}R, \tag{4}$$

$n \geq 0$,

$$v_{Y0}(R) = \sinh\left(\lambda_0 \frac{R}{R_\mathrm{d}}\right), \quad v_{Yn}(R) = \sin\left(\lambda_n \frac{R}{R_\mathrm{d}}\right), \quad n \geq 1,$$

$$||v_{Y0}||^2 = \int_0^{R_\mathrm{d}} v_{Y0}^2(R)\mathrm{d}R = -\frac{R_\mathrm{d}}{2}\left[1 + \frac{h_{Y0}}{h_{Y0}^2 - \lambda_n^2}\right], \tag{5}$$

$$||v_{Yn}||^2 = \int_0^{R_\mathrm{d}} v_{Yn}^2(R)\mathrm{d}R = \frac{R_\mathrm{d}}{2}\left[1 + \frac{h_{Y0}}{h_{Y0}^2 + \lambda_n^2}\right], \quad n \geq 1, \tag{6}$$

$$\alpha_m = \frac{|\dot{m}_\mathrm{d}|}{4\pi\rho_\mathrm{l} R_\mathrm{d}^2}, \tag{7}$$

$$\varepsilon_i = \frac{Y_{\mathrm{vs},i}}{\sum_i Y_{\mathrm{vs,i}}}. \tag{8}$$

When deriving (1) it was assumed that $\alpha_m = \text{const}$.

Note that there are typos in Eqs. (5.18) and (5.20) in [1] (Eqs. (1) and (4) in this article) which were corrected in [2].

In the case of a moving droplet the distribution for mass fractions of species can be described by the same Solution (1), but with D_l replaced by the effective diffusivity D_eff defined as [1]:

$$D_\mathrm{eff} = \chi_Y D_\mathrm{l}, \tag{9}$$

where the coefficient χ_Y can be approximated as:

$$\chi_Y = 1.86 + 0.86 \tanh\left[2.225 \log_{10}\left(\mathrm{Re}_{\mathrm{d(l)}}\mathrm{Sc_l}/30\right)\right], \tag{10}$$

$\mathrm{Sc_l} = \nu_\mathrm{l}/D_\mathrm{l}$ is the liquid Schmidt number, ν_l is the liquid kinematic viscosity. Liquid fuel transport properties and the liquid velocity just below the droplet surface were used to calculate $\mathrm{Re}_{\mathrm{d(l)}}$. The model based on Equations (9) and (10) is known as the Effective Diffusivity (ED) model.

Solution (1) with D_eff defined by (9) was used alongside the solutions for temperature and evaporation rate, summarised in [7], and Raoult's law to perform calculations for heating and evaporation of moving droplets [1].

3. Implementation of the model into ANSYS Fluent

Solution (1) for each species was implemented into the customised version of ANSYS Fluent alongside with the previously implemented equation for temperature distribution inside droplets [7]. The UDF supplied ANSYS Fluent with the right-hand-side terms in the heat and mass exchange equations. Thermodynamic and transport parameters were calculated based on the average temperature inside the droplets. The droplet volume was discretised into $N_\mathrm{L} = 500$ concentric layers to calculate the series in Solution (1) and in the corresponding solution for temperature distribution. The integrals and average temperatures inside droplets were also calculated using Simpson's method [9]. At each time step species distributions and temperatures were calculated from Solution (1) and the corresponding equation for temperature distribution. Time steps for calculations were taken equal to $\mathrm{d}t = 10^{-5}$ seconds. The roots of the eigenvalues were found using the bisection method with accuracy of 10^{-12}.

4. Results and discussions

The newly developed customised version of ANSYS Fluent was applied to the analysis of cooling and evaporation of droplets of mixture of ethanol and acetone, as described in the experiments the results of which are presented in [4]. The transport and thermodynamic properties of acetone and ethanol were taken from [4]. Three compositions of droplets were considered: 25% ethanol/75% acetone, 50% ethanol/50% acetone, 75% ethanol/25% acetone. Droplet initial temperatures and diameters, ambient gas temperatures and droplet velocities for each of these three cases are shown in Table 1.

Composition	T_{d0} (K)	d_0 (μm)	T_{g} (K)	v_{d} (m/s)
25% ethanol	305.65	133.8	294.25	12.75
50% ethanol	310.65	142.7	293.95	12.71
75% ethanol	311.75	137.1	294.75	12.28

Table 1: Droplet composition (percentage of ethanol), initial droplet temperature (T_{d0}), initial droplet diameter (d_0), gas temperature (T_{g}), and droplet velocity (v_{d}).

Note that in contrast to [4], we ignored the effects of interaction between droplets and the changes of droplet velocities with time. Taking into account both these effects would affect the values of predicted droplet temperatures and mass fractions, but would not affect the results of the comparison between the predictions of ANSYS Fluent and previously developed one-dimensional in-house code. The predictions of the latter code were verified against the predictions of the code based on the numerical solutions to the heat transfer and species diffusion equations [4]. This allows us to use the aforementioned code as the reference code to verify the results for heating and evaporation of droplets of various compositions predicted by the new customised version of ANSYS Fluent.

In all cases ambient gas pressure was taken equal to 100 kPa. Gas parameters in the vicinity of the droplet surface were calculated based on reference temperature $T_{\mathrm{ref}} = (2\,T_{\mathrm{s}} + T_{\mathrm{g}})/3$. 200 eigenvalues were used to calculate the temperature distribution and up to 100 eigenvalues were used to calculate the species mass fraction distributions (Solution (1)).

The results of the comparison between ANSYS Fluent and in-house code for the surface, centre and average temperatures of the droplet for a 25% ethanol and 75% acetone mixture are shown in Fig. 1. As follows from this figure, all three temperatures decrease with time, with surface temperature being always lower than that at the centre of the droplet, as expected. The difference between the temperatures at the centre and surface of the droplets reached up to 9 K, which cannot be ignored in most engineering applications. This difference was ignored in the conventional version of ANSYS Fluent, which cannot be justified in the general case.

The agreement between the predictions of ANSYS Fluent and in-house

Composition	Error (T_{d})	Error ($Y_{\mathrm{ls,e}}$)	Error ($Y_{\mathrm{ls,a}}$)
25% ethanol	0.1636%	0.3647%	0.1726%
50% ethanol	0.1423%	0.1730%	0.3110%
75% ethanol	0.1294%	0.2759%	0.7933%

Table 2: Droplet composition (percentage of ethanol), and maximal relative errors of estimation of droplet temperatures T_{d} (centre, surface and average droplet temperatures) and surface mass fractions of ethanol $Y_{\mathrm{ls,e}}$ and acetone $Y_{\mathrm{ls,a}}$. These errors were estimated as the ratios of the absolute values of the differences between the parameters predicted by ANSYS Fluent and the in-house code, divided by the values of parameters predicted by the in-house code.

codes is reasonably good with the maximal deviation between predicted temperatures not exceeding 0.1636% (see Table 2). This difference between the results can be ignored in almost all practical applications.

The plots for time evolution of ethanol and acetone mass fractions at the droplet surface, for the same conditions as those used for Fig. 1, are shown in Fig. 2. As follows from this figure, mass fraction of ethanol increases and mass fraction of acetone decreases during the evaporation process, as expected. Acetone is more volatile than ethanol and evaporates faster than ethanol. As in the case of temperatures, shown in Fig. 1, the agreement between the predictions of ANSYS Fluent and in-house code is good with the maximal deviation between predicted surface mass fractions not exceeding 0.3647% for ethanol and 0.1726% for acetone (see Table 2). This difference between the results can be ignored in almost all practical applications.

The deviations between the results predicted by ANSYS Fluent and the one-dimensional in-house code for 50% ethanol/50% acetone and 75% ethanol/25% acetone droplets turned out to be close to those shown in Figs. 1 and 2 (see Table 2). In all cases the changes in droplet radii were small and the corresponding curves are not shown.

The plots for temperature versus normalised distance from the droplet centre at three time instants for the same conditions as those used for Figs. 1 and 2 are shown in Fig. 3. As one can see from this figure, there is visible temperature gradient inside the droplet at all time instants under consideration. This is consistent with the results shown in Fig. 1. The agreement

between the predictions of ANSYS Fluent and the in-house code is reasonably good with the maximal deviation between predicted temperatures not exceeding 0.16% for $t = 4$ ms, 0.14% for $t = 5$ ms, and 0.13% for $t = 6$ ms. This difference between the results can be ignored in almost all practical applications.

Our analysis of the dependence of ethanol and acetone mass fractions on normalised distance from the droplet centre at various time instants led to the results consistent with those shown in Fig. 2. The deviation between the predictions of ANSYS Fluent and the in-house code were comparable with those shown in Fig. 2 and can be ignored in most practical applications.

We need to emphasise that we do not expect exact coincidence between ANSYS Fluent and in-house code results as most of numerical schemes used by ANSYS Fluent are not accessible for the users of this code.

Note that the results presented in the previous figures turned out to be rather sensitive to the choice of the number of terms in the series in Solution (1). To illustrate this sensitivity, the distribution of ethanol mass fraction inside the droplet ($Y_{\mathrm{l,e}}$) as the function of the normalised distance from the droplet centre, after the first time step (10^{-5} seconds), is shown in Fig. 4. As mentioned previously, in all calculations we used 100 terms in the series in (1). This case is shown by the solid curve in Fig. 4. The cases when this number of terms reduced to 40 and 10 are shown by the dashed and dotted curves, respectively, in the same figure.

As follows from Fig. 4, even in the case when 100 terms in the series in Solution (1) were used, there were deviations of the values of $Y_{\mathrm{l,e}}$ from 0.25 after the first time step both near the surface of the droplet and near its centre. The latter obviously does not have any physical meaning. In the case when this number of terms decreases to 40 this deviation becomes more pronounced especially near the centre of the droplet. In the case when this number of terms further decreases to 10, the distribution of $Y_{\mathrm{l,e}}$ inside the droplet and at its surface becomes unphysical. This justifies the use of 100 terms in the series in our analysis.

5. Conclusion

A model for heating and evaporation of multi-component droplets, based on analytical solutions to the heat transfer and species diffusion equations in the liquid phase, is summarised. The implementation of the model into ANSYS Fluent via User-Defined Function (UDF) is described. The model

is applied to the analysis of the mixtures of acetone/ethanol droplet heating/cooling and evaporation. The predictions of the customised version of ANSYS Fluent, with the new model implemented into it, are verified against the results predicted by the previously developed one-dimensional in-house code based on the analytical solutions to the heat transfer and mass diffusion equations. The agreement between the predictions of these codes is shown to be very good for multi-component droplets comprising acetone with 25, 50 and 75-percentage mass fractions of ethanol, with input parameters comparable with those used for previous verification and validation of the in-house code. This gives us confidence in using the new customised version of ANSYS Fluent for the analysis of more complex engineering processes involving droplet heating and evaporation.

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Figure Captions

Fig. 1 Time evolution of a 25% ethanol/75% acetone droplet surface (bottom curve), average (middle curve) and centre (top curve) temperatures ($T_{\rm s}$, $T_{\rm av}$ and $T_{\rm c}$) as predicted by the new customised version of ANSYS Fluent (solid curves) and previously developed one-dimensional in-house code (dashed curves).

Fig. 2 Time evolution of surface mass fractions of ethanol ($Y_{\rm ls,e}$) and acetone ($Y_{\rm ls,a}$) for a 25% ethanol/75% acetone droplet as predicted by the new customised version of ANSYS Fluent (solid) and previously developed one-dimensional in-house code (dashed).

Fig. 3 The plots of temperature versus normalised distance from the droplet centre for a 25% ethanol/75% acetone droplet at $t = 4$ ms (top curves), $t = 5$ ms (middle curves), and $t = 6$ ms (bottom curves), as predicted by the new customised version of ANSYS Fluent (solid) and previously developed one-dimensional in-house code (dashed).

Fig. 4 The plots of mass fractions of ethanol ($Y_{\rm l,e}$) versus normalised distance from the droplet centre for a 25% ethanol/75% acetone droplet after the first time step 10^{-5} seconds. Solid curve refers to the case when 100 of terms in Solution (1) were taken into account, dashed and dotted curves refer to the cases when 40 and 10 terms, respectively, in this solution were taken into account.

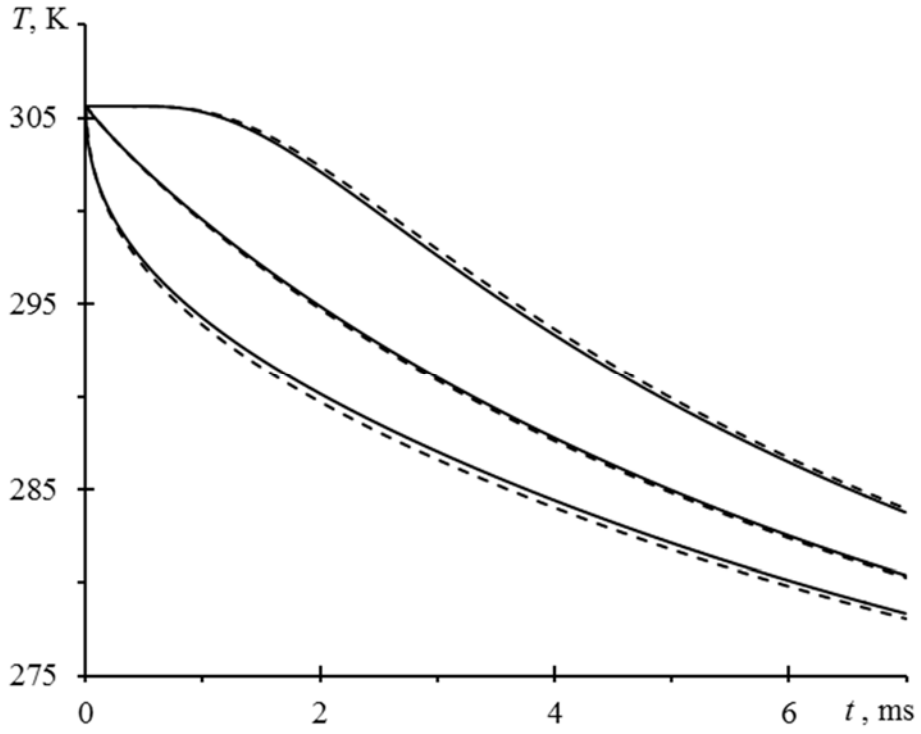

Figure 1

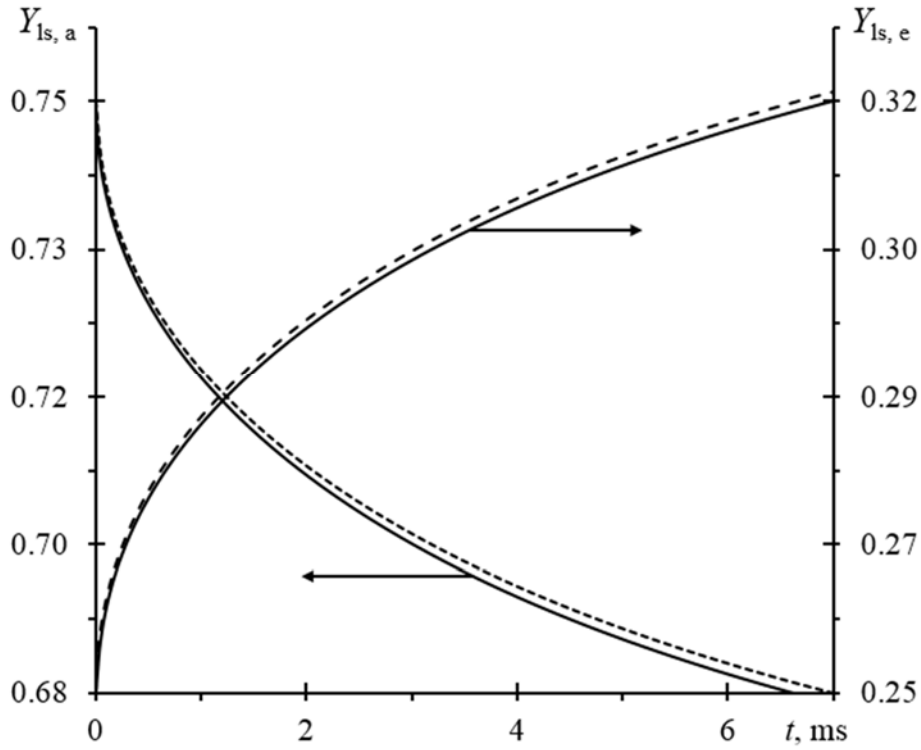

Figure 2

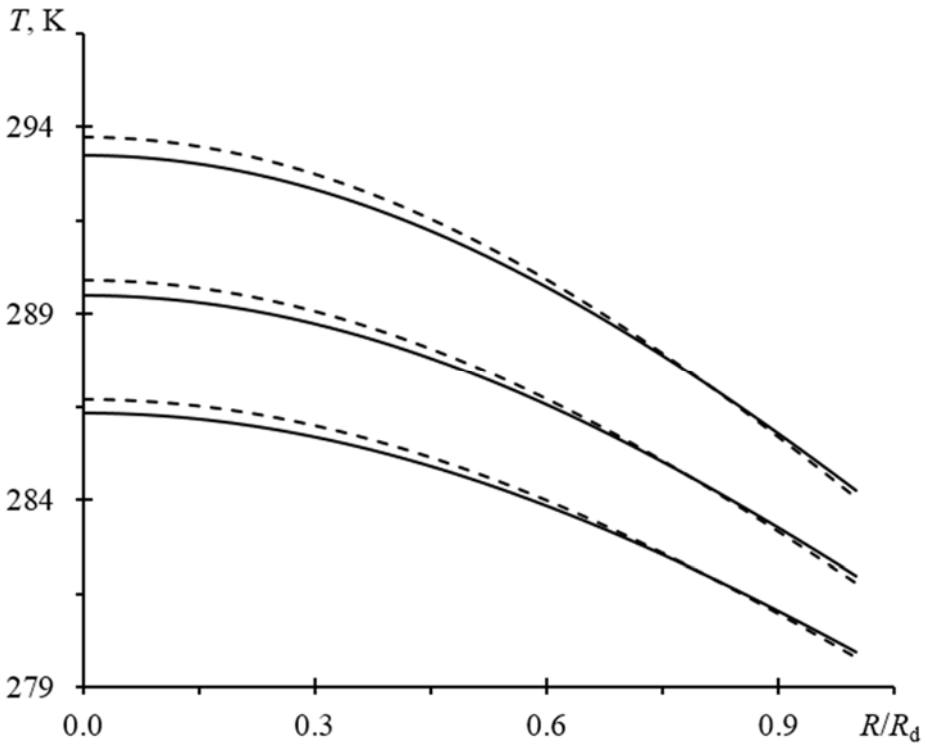

Figure 3

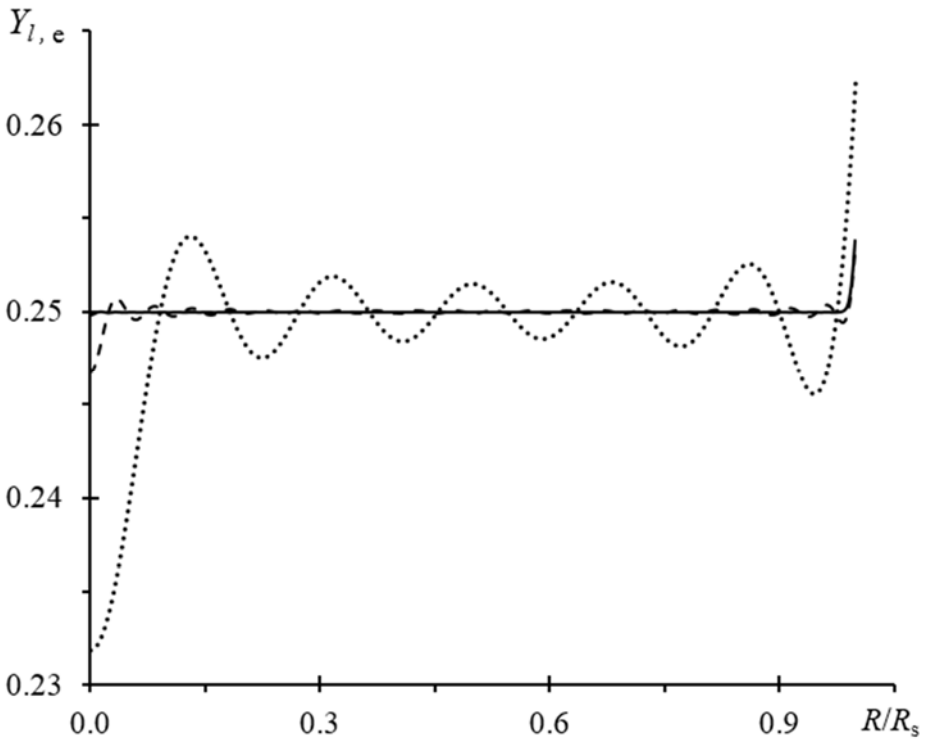

Figure 4