New solutions to the species diffusion equation inside droplets in the presence of the moving boundary

I.G. Gusev [a], P.A. Krutitskii [b], S.S. Sazhin [a,*], A.E. Elwardany [a]

[a] *Sir Harry Ricardo Laboratories, Centre for Automotive Engineering, School of Computing, Engineering and Mathematics, Faculty of Science and Engineering, University of Brighton, Brighton BN2 4GJ, UK*
[b] *Keldysh Institute for Applied Mathematics, Department 4, Miusskaya Sq. 4, Moscow 125047, Russia*

ABSTRACT

Two new solutions to the equation, describing the diffusion of species during multi-component droplet evaporation, are suggested. The first solution is the explicit analytical solution to this equation, while the second one reduces the solution of the differential transient species equation to the solution of the Volterra integral equation of the second kind. Both solutions take into account the effect of the reduction of the droplet radius due to evaporation, assuming that this radius is a linear function of time. The analytical solution has been incorporated into a zero dimensional CFD code and applied to the analysis of a bi-component droplet evaporation. The case of an initial 50% ethanol–50% acetone mixture and droplets with initial diameter equal to 142.7 μm moving in air at atmospheric pressure has been considered. To separate the effect of the moving boundary on the species diffusion equation from a similar effect on the heat conduction equation inside droplets, described earlier, a rather artificial assumption that the droplet temperature is homogeneous and fixed has been made. It has been pointed out that the effect of the moving boundary slows down the increase in the mass fraction of ethanol (the less volatile substance in the mixture) and leads to the acceleration of droplet evaporation.

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1. Introduction

The species diffusion equation, describing the dynamics of multi-component systems, its analysis and applications, has been widely discussed in the literature [1]. One of the most important applications of this equation is that to the analysis of evaporation of multi-component droplets [2,3]. In realistic moving droplets, species diffusion takes place alongside species convection when Hill-type vortices are formed inside droplets [4]. In most practically relevant cases, however, the details of species distribution inside droplets are not important and the effects of species diffusion and convection can be described in terms of the spherically symmetric effective diffusivity model [3]. In [5] this model was applied to the analysis of heating and evaporation of bi-component ethanol/acetone droplets. In contrast to the previous studies of these processes, the authors of [5] based their analysis on the analytical solution to the species diffusion equation, which was incorporated into the numerical code, rather than on the numerical solution of this equation. This approach is expected to be more CPU efficient and accurate compared with the one based on the conventional approach [6]. The model described in [5] has been generalised in [7] to take into account coupling between droplets and gas.

Following its wide use in Computational Fluid Dynamics (CFD) codes, the droplet radius was assumed to be constant during each time step, but changes from one time step to another were allowed to take into account droplet evaporation. As shown in [8–10], in the case of the thermal conduction equation inside droplets this approach leads to noticeable overestimation of droplet surface temperature and underestimation of its evaporation time, compared with the approach in which the change in droplet radius during the time step is ignored.

The main purpose of this paper is to generalise the analytical solution to the species diffusion equation, reported in [5,7], to the case when the changes in droplet radius during the time steps are taken into account. This new solution will be applied to the analysis of bi-component droplet evaporation. The importance of taking into account the changes in droplet radius during the time step will be investigated.

Basic equations and approximations used in our analysis are presented and discussed in Section 2. The details of the new analytical solution of the species diffusion equation are given in Section 3. In Section 4 this solution is applied to the analysis of bi-component droplet evaporation. The main results of the paper are summarised in Section 5.

* Corresponding author. Tel.: +44 (0) 1273642677; fax: +44 (0) 1273642309.
 E-mail address: S.Sazhin@brighton.ac.uk (S.S. Sazhin).

Nomenclature

B_M	Spalding mass transfer number		α_m	parameter defined by Eq. (3)
C_F	friction drag coefficient		γ	activity coefficient
D	diffusion coefficient		ϵ	evaporation rate
f	function defined by Eq. (32)		Θ	function introduced in Eq. (24)
F	function introduced in Eq. (13) or (16)		$\bar{\Theta}$	function defined by Eq. (46)
G	function introduced in Eq. (53)		λ, λ_n	eigenvalues defined by Eq. (28) or (30)
h_0	function introduced in Eq. (21)		$\mu_0(t)$	variable introduced in Eq. (20)
H_0	function introduced in Eq. (20)		$\hat{\mu}_0(t)$	variable introduced in Eq. (51)
h_1	function introduced in Eq. (50)		v	kinematic viscosity
L	latent heat of evaporation		ξ	R/R_d
m	mass		ρ	density
M	molar mass		χ_Y	parameter defined by Eq. (7)
p	pressure or parameter introduced in Eq. (25)			
q_n	parameter introduced in Eq. (33)		*Subscripts*	
R	distance from the droplet centre		a	air
R_d	droplet radius		amb	ambient
R_u	universal gas constant		b	boiling
Re	Reynolds number		d	droplet
Sc	Schmidt number		eff	effective
Sh	Sherwood number		eth	ethanol
t	time		i	species
U_s	maximal surface velocity		iso	isolated
v_n	eigenfunctions of (25)		l	liquid
V	function introduced in Eq. (22)		part	particular
$\mathcal{V}$	function introduced in Eq. (53)		s	surface
W	function introduced in Eq. (16)		v	vapour
X	molar fraction		0	initial
Y	mass fraction		∞	ambient conditions
Greek symbols				
α	parameter introduced in Eq. (4)			

2. Basic equations and approximations

Assuming that all processes inside droplets are spherically symmetric (droplets are stationary), the equations for mass fractions of liquid species $Y_{li} \equiv Y_{li}(t,R)$ inside multi-component droplets can be presented in the following form [3]:

$$\frac{\partial Y_{li}}{\partial t} = D_l \left(\frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R}\frac{\partial Y_{li}}{\partial R} \right), \tag{1}$$

where $i > 1$, D_l is the liquid mass diffusivity. $Y_{li}(t,R)$ is a twice continuously differentiable function. Eq. (1) needs to be solved with the following boundary condition [3]:

$$\alpha_m(\epsilon_i - Y_{lis}) = -D_l\frac{\partial Y_{li}}{\partial R}\bigg|_{R=R_d(t)-0} \tag{2}$$

and the initial condition $Y_{li}(t = 0) = Y_{li0}(R)$, where $Y_{lis} = Y_{lis}(t)$ are liquid components' mass fractions at the droplet's surface,

$$\alpha_m = \frac{|\dot{m}_d|}{4\pi\rho_l R_d^2}, \tag{3}$$

ϵ_i is the evaporation rate of species.

Note that $0 \leqslant Y_{li} \leqslant 1$ due to the physical nature of this parameter.

We assume that $R_d(t)$ is the linear function of t during each time step:

$$R_d(t) = R_{d0}(1 + \alpha t), \tag{4}$$

where $\alpha = -\alpha_m/R_{d0}$.

Although α_m and α are linked by a simple relation, it is important for us to retain the difference between these two parameters.

α_m describes the rate of removal of species from the surface of the droplet, while α describes the rate of change in droplet radius during time steps. The latter effect was ignored in most previous analysis of this phenomenon, including [5,7], where it was assumed that $\alpha = 0$, but $\alpha_m \neq 0$ was still defined by Eq. (3). In our analysis both these effects are taken into account.

Assuming that species concentrations in the ambient gas are equal to zero ($Y_{vi\infty} = 0$), the values of ϵ_i can be found from the following relation [5]:

$$\epsilon_i(t) = \frac{Y_{vis}}{\sum_i Y_{vis}}, \tag{5}$$

where the subscript v indicates the vapour phase. We assume that ϵ_i are still defined by Eq. (5) even in the case when these concentrations are not equal to zero. Eq. (1) can be generalised to take into account the effect of moving droplets with the help of the effective diffusivity model [3] in which D_l in Eq. (1) is replaced with

$$D_{\text{eff}} = \chi_Y D_l, \tag{6}$$

where the coefficient χ_Y varies from 1 to 2.72 and can be approximated as:

$$\chi_Y = 1.86 + 0.86\tanh[2.245\log_{10}(\text{Re}_l\text{Sc}_l/30)], \tag{7}$$

Sc_l is the liquid Schmidt number defined as:

$$\text{Sc}_l = \frac{v_l}{D_l}, \tag{8}$$

v_l is the liquid kinematic viscosity, Re_l is the Reynolds number based on droplet radius, liquid transport properties and the maximum surface velocity inside droplets. The latter velocity was calculated as [11]: