International Communications in Heat and Mass Transfer 90 (2018) 29–33

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

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

O. Rybdylova[a,*], L. Poulton[a], M. Al Qubeissi[b], A.E. Elwardany[c], C. Crua[a], T. Khan[a,d], S.S. Sazhin[a]

[a] Sir Harry Ricardo Laboratories, Advanced Engineering Centre, School of Computing, Engineering and Mathematics, University of Brighton, Brighton BN2 4GJ, United Kingdom
[b] Centre for Mobility & Transport, Faculty of Engineering, Environment and Computing, Coventry University, Coventry CV1 2JH, United Kingdom
[c] Mechanical Engineering Department, Faculty of Engineering, Alexandria University, Alexandria 21544, Egypt
[d] Institute of Space Technology, P.O. Box 2750, Islamabad 44000, Pakistan

ARTICLE INFO

Keywords:
Droplets
Heating
Evaporation
ANSYS Fluent
Ethanol
Acetone

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.

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 reported 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

* Corresponding author.
E-mail address: O.Rybdylova@brighton.ac.uk (O. Rybdylova).

https://doi.org/10.1016/j.icheatmasstransfer.2017.10.018

Nomenclature

d	Diameter of a droplet
D	Diffusion coefficient
$h_{Y\,0}$	Parameter defined by Eq. (2)
$\dot{m}$	Evaporation rate
N_{L}	Number of layers inside a droplet
Pe	Peclet number
Pr	Prandtl number
$q_{Y\,in}$	Parameter defined by Eq. (4)
$Q_{Y\,n}$	Parameter defined by Eq. (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
$v_{Y\,n}$	Eigenfunction
Y	Mass fraction

Greek symbols

α_m	Parameter defined by Eq. (7)
ε_i	Parameter defined by Eq. (8)
λ_n	Eigenvalues
ν	Kinematic viscosity
ρ	Density
χ_Y	Correction function defined by Eq. (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

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_{d} is constant (an approximation valid for short time steps), the analytical solution to this equation for the mass fractions $Y_{1,i}$, subject to the initial condition $Y_{1,i}(t=0,R) = Y_{1,i0}(R)$, is presented as [1]

$$Y_{l,i} = \varepsilon_i + \frac{1}{R}\left\{\exp\left[D_{\mathrm{l}}\left(\frac{\lambda_0}{R_{\mathrm{d}}}\right)^2 t\right][q_{Yi0} - Q_{Y0}\varepsilon_i]\sinh\left(\lambda_0\frac{R}{R_{\mathrm{d}}}\right) + \sum_{n=1}^{\infty}\left[\exp\left[-D_{\mathrm{l}}\left(\frac{\lambda_n}{R_{\mathrm{d}}}\right)^2 t\right][q_{Yin} - Q_{Yn}\varepsilon_i]\sin\left(\lambda_n\frac{R}{R_{\mathrm{d}}}\right)\right]\right\}, \tag{1}$$

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

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

respectively,

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

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

$$q_{Yin} = \frac{1}{||v_{Yn}||^2}\int_0^{R_{\mathrm{d}}} R Y_{\mathrm{li0}}(R) v_{Yn}(R)\mathrm{d}R, \tag{4}$$

$n \geq 0$,

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

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

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

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

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

When deriving Eq. (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

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

$\mathrm{Sc_l} = \nu_{\mathrm{l}}/D_{\mathrm{l}}$ 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 Eqs. (9) and (10) is known as the Effective Diffusivity (ED) model.

Solution (1) with D_{eff} defined by Eq. (9) was used alongside the