International Communications in Heat and Mass Transfer 76 (2016) 265–270

Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

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

A model for droplet heating and its implementation into ANSYS Fluent☆

O. Rybdylova[a,*], M. Al Qubeissi[a,b], M. Braun[c], C. Crua[a], J. Manin[d], L.M. Pickett[d], G. de Sercey[a], E.M. Sazhina[a], S.S. Sazhin[a], M. Heikal[a]

[a]Sir Harry Ricardo Laboratories, School of Computing, Engineering and Mathematics, University of Brighton, Brighton BN2 4GJ, United Kingdom
[b]Centre for Mobility & Transport, School of Mechanical, Aerospace and Automotive Engineering, Coventry University, Coventry CV1 2JH, United Kingdom
[c]ANSYS Germany GmbH, Darmstadt 64295, Germany
[d]Sandia National Laboratories, 7011 East Avenue, 94550 Livermore, CA, United States

ARTICLE INFO

Available online 26 May 2016

Keywords:
Droplets
Heating
Evaporation
ANSYS Fluent
Diesel fuel
n-Dodecane

ABSTRACT

The main ideas of the model for droplet heating and evaporation, based on the analytical solution to the heat conduction equation inside the droplet, and its implementation into ANSYS Fluent are described. The model is implemented into ANSYS Fluent using User-Defined Functions (UDF). The predictions of ANSYS Fluent with the new model are verified against the results predicted by in-house research code for an *n*-dodecane droplet heated and evaporated in hot air. Also, the predictions of this version of ANSYS Fluent are compared with in-house experimental data.

1. Introduction

A new model for multi-component droplet heating and evaporation, based on the analytical solutions to the heat transfer and species diffusion equations, has been developed by our group (see Refs. [1,2] for the details). This model has been validated based on the available experimental data and the predictions of the numerical codes using the analytical solution to these equations [3,4].

In the current study the analysis is restricted to mono-component droplets. The main ideas of the new model and the results of its implementation into the commercial CFD code ANSYS Fluent, via User-Defined Functions (UDF), macros, supported by ANSYS Fluent, are summarised. The results of the implementation of the model are compared with the predictions of the in-house code and validated against in-house experimental data.

The mathematical formulation and the implementation of the model are described in Section 2. In Section 3.1, the predictions of ANSYS Fluent with the new model are verified against the predictions of the in-house code. In Section 3.2, the experimental set-up is described, and the results of simulations are compared with the experimental data. The main results of the paper are summarised in Section 4.

2. Formulation of the problem

In the conventional approach, used in most available CFD codes, including ANSYS Fluent, droplet heating is modelled based on the solution to the following energy balance equation:

$$c_{pl} m_d \frac{dT}{dt} = 2\pi \mathrm{Nu} k_g R_d (T_g - T_s) + L\dot{m}_d + q_{\mathrm{int}}, \quad (1)$$

where c_{pl} is droplet liquid specific heat capacity, m_d and R_d are droplet mass and radius, respectively, Nu is the Nusselt number, k_g is gas thermal conductivity, T_g and T_s are gas and surface temperatures, respectively, L is the latent heat of evaporation, q_{int} is heat supplied or removed from internal sources (e.g. chemical reactions). The derivation of this equation is based on the assumption that the effects of temperature gradients inside droplets can be ignored. This assumption is commonly supported by the fact that liquid thermal conductivity is much higher than gas thermal conductivity in most engineering applications. At the same time, when modelling transient processes this assumption should be based on the comparison of the liquid and gas thermal diffusivities and the values of the Fourier number. In most engineering applications, including Diesel engines, liquid thermal diffusivities are much lower than

☆ Communicated by J. Rose and A. Briggs.
* Corresponding author.
E-mail address: O.Rybdylova@brighton.ac.uk (O. Rybdylova).

http://dx.doi.org/10.1016/j.icheatmasstransfer.2016.05.032
0735-1933/

Nomenclature

B_M, B_T	Spalding mass and heat transfer numbers
c_p	specific heat capacity at constant pressure
D	binary diffusivity coefficient of vapour in air
h	convection heat transfer coefficient
I_n	integrals, used in series (2) and (6)
j	parameter, defined in Eq. (4b)
k	thermal conductivity
L	latent heat of evaporation
m	mass
$\dot{m}$	evaporation rate
M	molar mass
N_L	number of layers inside a droplet
Nu	Nusselt number
Pe	Peclet number
p	pressure
Pr	Prandtl number
q	heat flux
r	radial coordinate from the centre of the droplet
R_d	radius of a droplet
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
t	time
T	temperature
$\mathbf{v}$	velocity
Y	mass fraction
x	molar fraction

Greek symbols

κ	parameter defined by Eq. (4a)
λ_n	eigenvalues defined by Eq. (3)
μ	dynamic viscosity
ρ	density
ϕ	parameter defined by Eq. (5e)
χ	correction function defined by Eq. (4b)
ζ	parameter defined by Eq. (4a)

Subscripts

d	droplet
eff	effective
g	gas
int	internal
l	liquid
ref	reference value
s	surface of droplet
sat	saturation
t	total
v	vapour
0	value at the beginning of a time step
∞	value in the far field

those of gas. This obviously brings into question the applicability of Eq. (1). This equation cannot be used at all when the Fourier numbers are small.

In an alternative approach to the problem of droplet heating, taking into account the effects of temperature gradient inside droplets, the transient heat conduction inside the droplet is solved subject to the boundary conditions at the surface of the droplet. Assuming that all the processes inside the droplet are spherically symmetric, an analytical solution to this equation during any time step Δt ($t \in [0, \Delta t]$) has been found in the form [2,4]:

$$T(r,t) = \frac{1}{r}\sum_{n=1}^{\infty}\left\{\left(I_n - \frac{R_d \sin\lambda_n}{\lambda_n^2}\zeta(0)\right)\frac{\exp\left(-\kappa\lambda_n^2 t\right)}{b_n} - \right.$$
$$\left. - \frac{R_d \sin\lambda_n}{b_n\lambda_n^2}\int_0^t \frac{d\zeta(\tau)}{d\tau}\exp\left(-\kappa\lambda_n^2(t-\tau)\right)d\tau\right\}$$
$$\sin\left(\lambda_n\frac{r}{R_d}\right) + T_{\text{eff}}(t), \tag{2}$$

where λ_n are positive roots to the eigenvalue equation

$$\lambda\cos\lambda + j\sin\lambda = 0; \tag{3}$$

in ascending order,

$$b_n = \frac{1}{2}\left(1 + \frac{j}{j^2+\lambda_n^2}\right),\ I_n = \int_0^{R_d}\frac{r}{R_d}T_0(r)\sin\left(\lambda_n\frac{r}{R_d}\right)dr,$$

$T_0(r)$ is the initial temperature distribution inside the droplet or the distribution predicted at the previous time step;

$$\kappa = \frac{k_{\text{eff}}}{c_{pl}\rho_l R_d^2},\ \zeta(t) = \frac{hT_{\text{eff}}(t)R_d}{k_{\text{eff}}},\ T_{\text{eff}} = T_g + \frac{\dot{m}_d L}{2\pi R_d \text{Nu} k_g}; \tag{4a}$$

$$j = \frac{hR_d}{k_{\text{eff}}} - 1,\ h = \frac{k_g \text{Nu}}{2R_d},\ k_{\text{eff}} = \chi k_l,$$
$$\chi = \left(1.86 + 0.86\ \tanh\left(2.225\quad \lg\frac{\text{Pe}}{30}\right)\right), \tag{4b}$$

$$\text{Pe} = 0.79\left|\mathbf{v}_g - \mathbf{v}_d\right|\frac{\mu_g}{\mu_l}\frac{\text{Re}_d^{1/3}}{1+B_M}\frac{\rho_l R_d c_{pl}}{k_l},\ \text{Re}_d = \frac{2R_d\rho_g\left|\mathbf{v}_g - \mathbf{v}_d\right|}{\mu_g}, \tag{4c}$$

where $B_M = (Y_{vs} - Y_{v\infty})/(1 - Y_{vs})$, $Y_{v\infty}$ and Y_{vs} are mass fractions of vapour in the ambient gas and at the droplet surface. Note that

$$Y_{vs} = \frac{x_{vs}M_v}{x_{vs}M_v + (1-x_{vs})M_a},\ x_{vs} = \frac{p_{sat}}{p}.$$

The Nusselt number is approximated as [2]:

$$\text{Nu} = \frac{\ln(1+B_T)}{B_T}\text{Nu}^*, \tag{5a}$$

$$\text{Nu}^* = 2 + \frac{(1+\text{Re}_d\,\text{Pr})^{1/3}\max\left(1,\text{Re}_d^{0.077}\right) - 1}{F(B_T)}, \tag{5b}$$

$$\text{Sh}^* = 2 + \frac{(1+\text{Re}_d\text{Sc})^{1/3}\max\left(1,\text{Re}_d^{0.077}\right) - 1}{F(B_M)}, \tag{5c}$$

$$F(B_{T,M}) = (1+B_{T,M})^{0.7}\frac{\ln(1+B_{T,M})}{B_{T,M}},\ B_T = (1+B_M)^{\phi} - 1, \tag{5d}$$

$$\phi = \frac{c_{pv}\rho_g D}{k_g}\frac{\text{Sh}^*}{\text{Nu}^*},\ \text{Pr} = \frac{c_{pg}\mu_g}{k_g},\ \text{Sc} = \frac{\mu_g}{\rho_g D}. \tag{5e}$$