International Journal of Heat and Mass Transfer 92 (2016) 184–189

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

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

A multi-component drop evaporation model based on analytical solution of Stefan–Maxwell equations

S. Tonini, G.E. Cossali *

Department of Engineering and Applied Sciences, University of Bergamo, Viale Marconi 5, 24044 Dalmine, Italy

ARTICLE INFO

Article history:
Received 8 June 2015
Received in revised form 4 August 2015
Accepted 4 August 2015
Available online 10 September 2015

Keywords:
Multi-component drop evaporation
Stefan–Maxwell equations
Fick's law approximation

ABSTRACT

A novel evaporation model for multi-component spherical drop has been developed by analytically solving the Stefan–Maxwell equations under spherical symmetry assumptions. The evaporation rate predicted by the new model is compared with the predictions obtained by previous models based on Fick's law approximation, under steady-state isothermal conditions for a wide range of gas and drop temperatures and compositions. The effect of non-isothermal conditions are considered in a simplified way, through the effect of temperature on the reference value of gas density and mass diffusion coefficients. The Fick's law based models are found to generally under-predict the total evaporation rate, particularly at higher evaporation rate conditions.

1. Introduction

In many applied fields, like spray combustion, spray painting, aerosol for medical applications, etc., the evaporation of a liquid drop floating in a gaseous atmosphere is a phenomenon of paramount importance. Since the early work of Maxwell on this subject [1], back in 1877, a relatively vast literature has become available, reporting the valuable findings that helped to increase our understanding of the complex phenomena involved. During the evaporation of a liquid drop different simultaneous mechanisms of heat (conduction, convection and possibly radiation) and mass (convection and diffusion) transfer, between the drop surface and the surroundings, influence and drive the drop evaporation (see [2] for a detailed description).

A wide literature is available on the modelling of the above mentioned phenomena, (see for example [3,4] for a review), particularly for a single component drop, and such models are often used to simulate evaporating spray, as part of CFD methodologies, although detailed models based on single drop analysis have to be simplified to be CPU efficient.

A far less amount of literature is available on the more complex problem of evaporation from a multi-component droplet, since in this case the simultaneous diffusive–convective mass transfer from the drop to the gas cannot be simply modelled and/or experimentally studied. The Stefan flow combined with the differential diffusion of each component into the gas–vapour mixture renders the problem much more complex than that relative to single component drops. A typical approach to this problem is to model the diffusive mass flux of each component by the well-known Fick's law, which however would exactly hold only for binary diffusion (i.e. single component vapour diffusing in a gas) [5].

The available studies on multi-component diffusion from spherical drops are based on the simplified extension of single component models (namely the Fuchs' model [6] for evaporation in a still gas and the Abramzon and Sirignano extension [7] to $Re > 0$), with different simplifying conditions. A typical simplification is to consider the vapour mixture as a single component, defining an average diffusive coefficient into the gaseous atmosphere, that can be done in different ways. For example, Sazhin et al. [8] proposes to evaluate the diffusion coefficient of the mean vapour mixture in air according to the Wilke formula [9], which takes into account the physical properties of each species.

A slightly more detailed numerical model accounts for the difference between the diffusion coefficient of each species, thus evaluating the evaporation rate of each component [10]. Another similar approach was suggested by Brenn et al. [11] to account for differential diffusion of each component, namely the application of the single component model using an equivalent drop radius for each component, based on the volume composition of the real drop. Recently, Tonini and Cossali [12] proposed an analytical model of multi-component drop evaporation accounting for the inter-species mass diffusion in the gaseous mixture and suggested a simpler model, based on the single-component analogy, with a new definition of the mean mass diffusion coefficient, which results were found to be in good agreement with

* Corresponding author.
E-mail address: cossali@unibg.it (G.E. Cossali).

http://dx.doi.org/10.1016/j.ijheatmasstransfer.2015.08.014
0017-9310/

Nomenclature

$\mathcal{A}$	coefficient matrix (–)
$\mathbf{B}$	source term vector (–)
$\mathbf{C}_0$	constant of integration vector (–)
c	molar density (kmol/m^3)
D	species diffusion coefficient (m^2/s)
$\mathcal{I}$	unit matrix (–)
m_{ev}	evaporation rate (kg/s)
M_m	molar mass (kg/kmol)
$\mathbf{n}$	mass flux vector (kg/m^{2}s)
$\mathbf{N}$	molar flux vector (kmol/m^{2}s)
N_{ev}	molar evaporation rate (kmol/s)
N_r	molar flux vector radial component (kmol/m^{2}s)
r	radial coordinate (m)
R	universal gas constant (J/kmol K)
R_0	drop radius (m)
T	temperature (K)
y	molar fraction (–)

Greek symbols

ε	mass evaporation rate fraction (–)
ζ	non-dimensional coordinate (–)
v	molar evaporation rate fraction (–)
ρ	mass density (kg/m^3)
φ	species diffusion coefficient ratio (–)
χ	mass fraction (–)
Ψ	molar fraction vector (–)

Subscripts

ev	evaporation
ref	reference
s	drop surface
v	vapour
∞	ambient conditions

Superscripts

F	Fick model
j, k, n, p	indexes
m	mixture
T	total
$\hat{}$	non-dimensional

the more accurate solution. Ebrahimian and Habchi [13] developed a multi-component drop evaporation model, which proposes a new expression to evaluate the Stefan velocity based on [14], implementing it in a numerical code to compare the predictions with previous models and with available experimental results. The model was used to investigate the effect on drop evaporation rate of various model assumptions, like the infinite thermal conductivity assumption [3], the physical property averaging [15], the effect of high pressure and temperature conditions [16] and of gravity and natural convection [17–20].

All the previously mentioned models are based on the Fick's law approximation, although a more accurate way to cope with multi-component diffusion is through the so-called Stefan–Maxwell equations (see [5] for a comprehensive analysis), that can account for the mutual interaction among the mass fluxes of all the components. The major complexity of this approach comes from the fact that a system of coupled differential equations (one for each component) must be solved, together with continuity equations.

The next sections describe the mathematical formulation of a new model for drop evaporation based on the analytical solution of Stefan–Maxwell equations, under some simplifying hypotheses. A comparison with results obtained with previous models are reported. Finally the main conclusions arisen from the present investigation are briefly summarised.

2. Model equations

Steady multi-component diffusion can be correctly modelled by the Stefan–Maxwell (S–M) equations, that can be written, for a mixture of $n+1$ species, neglecting Soret effect and diffusion due to pressure gradients and to external force, as [5]:

$$\nabla y^{(p)} = \sum_{k=0}^{n} \frac{1}{cD_{pk}} \left(y^{(p)} \mathbf{N}^{(k)} - y^{(k)} \mathbf{N}^{(p)} \right) \tag{1}$$

where c is the molar density, $D_{pk} = D_{kp}$ are the binary diffusion coefficient of p-component into k-component, $y^{(p)}$ is the molar fraction of p-component, $\mathbf{N}^{(p)}$ is the molar flux of the p-component, which is related to the mass flux by $\mathbf{n}^{(p)} = \mathbf{N}^{(p)} Mm^{(p)}$ where $Mm^{(p)}$ is the molar mass of the p-component.

Considering a multi-component spherical drop evaporating in a gaseous atmosphere, spherical symmetry assumption allows to retain only the radial component of the species molar fluxes ($N_r^{(k)}$). Assuming a still drop surface and a neglectful gas diffusion into the liquid drop, the gas flux ($N_r^{(0)}$) is necessarily nil everywhere, then:

$$N_r^{(k)} = \frac{N_{ev}^{(k)}}{4\pi r^2} \quad \text{for} \quad k = 1 \dots n$$
$$N_r^{(0)} = 0$$

where $N_{ev}^{(k)}$ is the molar evaporation rate of the k-component (again $m_{ev}^{(k)} = N_{ev}^{(k)} Mm^{(k)}$, where $m_{ev}^{(k)}$ is the evaporation mass rate).

With the change of variable $\zeta = \frac{R_0}{r}$ and introducing the non-dimensional molar evaporation rate $\hat{N}_{ev}^{(k)} = \frac{N_{ev}^{(k)}}{4\pi R_0 c D_{ref}}$, where D_{ref} is a suitable reference value for the diffusion coefficients, Eq. (1) yields the ODE system:

$$\frac{dy^{(p)}}{d\zeta} = -\hat{N}_{ev}^{(T)} \sum_{k=0}^{n} \varphi^{pk} \left(y^{(p)} v^{(k)} - y^{(k)} v^{(p)} \right) \tag{2}$$

where $\varphi^{pk} = \frac{D_{ref}}{D_{pk}}$ and $v^{(k)} = \frac{N_{ev}^{(k)}}{\sum_{p=1}^{n} N_{ev}^{(p)}}$. Since $v^{(0)} = 0$ and $\sum_{k=0}^{n} y^{(k)} = 1$ and setting $\varphi^{pp} \equiv \varphi^{0p} \equiv \varphi^{p0}$ the system (2) can be written in matrix form as:

$$\frac{d}{d\zeta} \Psi = \mathcal{A} \Psi + \mathbf{B} \tag{3}$$

where

$$\mathcal{A} = \hat{N}_{ev}^{(T)} \begin{bmatrix} -\sum_{k=1}^{n} \varphi^{1k} v^{(k)} & v^{(1)} \left(\varphi^{12} - \varphi^{10} \right) & \dots & v^{(1)} \left(\varphi^{1n} - \varphi^{10} \right) \\ v^{(2)} \left(\varphi^{21} - \varphi^{20} \right) & -\sum_{k=1}^{n} \varphi^{2k} v^{(k)} & \dots & v^{(2)} \left(\varphi^{2n} - \varphi^{20} \right) \\ \dots & \dots & \dots & \dots \\ v^{(n)} \left(\varphi^{n1} - \varphi^{n0} \right) & v^{(n)} \left(\varphi^{n2} - \varphi^{n0} \right) & \dots & -\sum_{k=1}^{n} \varphi^{nk} v^{(k)} \end{bmatrix} \tag{4}$$