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A new model for a drying droplet

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ABSTRACT

A new model for droplet drying is suggested. This model is based on the analytical solutions to the heat transfer and species diffusion equations inside spherical droplets. Small solid particles dispersed in an ambient evaporating liquid, or a non-evaporating substance dissolved in this liquid, are treated as non-evaporating components. Three key sub-processes are involved in the process of droplet drying within the new model: droplet heating/cooling, diffusion of the components inside the droplets, and evaporation of the volatile component. The model is used to analyse the drying of a spray consisting of chitosan dissolved in water. After completion of the evaporation process, the size of the residual solid ball predicted by the model is consistent with those observed experimentally.

1. Introduction

The importance of spray/droplet drying in various engineering and pharmaceutical applications is well known [1–4]. Spray-drying technology can be utilised to incorporate different excipients as well as active pharmaceutical ingredients into a dry powder formulations. A few advantages include modification of the aerosolisation characteristics of the spray-dried powder [5,6], and sustained release of the active drug using appropriate modifiers such as hydroxypropyl cellulose [7] and polylactic acid [8]. Reviews of particle engineering via spray drying were presented by Vehring [9] and Yan Wei [10]. Various aspects of, and recent advances in spray drying are presented in [11]. Mezhericher et al. [12] reviewed theoretical studies of slurry droplet evaporation kinetics.

Mathematical models of the evaporation of slurry droplets of various complexity were developed by a number of authors, including [1,4,13–18]. A simplified model for evaporation of slurry droplets was developed by Minoshima et al. [19].

These models have been based on a number of simplifying assumptions, including the assumption that the temperature gradient inside droplets can be ignored. The applicability of these assumptions has not been investigated in most cases. The main aim of this paper is to present the results of the development of a new model for spray drying which relaxes many of the previously used assumptions and takes into account the gradients of small solid particle or dissolved non-evaporating substance concentrations and temperature inside droplets in a self-consistent way.

The new model is based on the model for automotive fuel droplet heating and evaporation, previously developed by one of the authors (SSS) and his colleagues (see [20,21]). In this model, small solid particles dispersed in an ambient evaporating liquid, or a non-evaporating substance dissolved in this liquid, are treated as non-evaporating components. Analytical solutions to the equations for species diffusion and heat transfer inside droplets are used for the analysis of the process at each time step. The model is applied to the process of spray drying to produce chitosan particles.

Basic equations and assumptions of the model are described in Section 2. The technology involved in the preparation of chitosan particles and input parameters to the model are described in Section 3. The solution algorithm is briefly described in Section 4. Results of calculations, based on the new model and using input parameters described in Section 3, are presented and discussed in Section 5. The main results of the paper are summarised in Section 6.

2. Model

The model is focused on the analysis of heating and evaporation of droplets with small solid particles dispersed in an ambient

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Nomenclature

$B_{M(T)}$	Spalding mass (heat) transfer number
c	specific heat capacity
D	diffusion coefficient
F	function introduced in Eq. (7)
h	convection heat transfer coefficient
h_0	parameter introduced in Eq. (2)
h_{0Y}	parameter introduced in Eq. (10)
k	thermal conductivity
k_B	Boltzmann constant
L	specific heat of evaporation
Le	Lewes number
M	molar mass
$\dot{m}_d$	evaporation mass rate
Nu	Nusselt number
p	pressure
Pe	Peclet number
Pr	Prandtl number
q_n	parameter introduced in Eq. (2)
q_{Yin}	parameter defined by Eq. (12)
Q_L	power spent on droplet heating
Q_{Yn}	parameter defined in Eq. (11)
R	distance from the droplet centre
R_d	droplet radius
Re	Reynolds number
Sc	Schmidt number
t	time
T^*	normalised temperature
T	temperature
v	velocity
v_n, v_{Yn}	eigenfunctions
V_v	parameter defined in Eq. (22)
X	molar fraction
Y	mass fraction

Greek symbols

α	film parameter defined in Eq. (9)
ϵ_i	evaporation rate of species i
$\varepsilon_{v(a)}$	characteristic Lennard-Jones energy for vapour (air)
κ_R	parameter introduced in Eq. (2)
λ_n	eigenvalues
μ	dynamic viscosity
μ_0	parameter introduced in Eq. (2)
ν	kinematic viscosity
ρ	density
σ_v	Lennard-Jones length
χ	coefficient defined in Eq. (5)
χ_Y	coefficient defined in Eq. (14)
Ω_D	parameter introduced in Eq. (24)

Subscripts

air	air
av	average
c	centre
d	droplet
eff	effective
e	evaporation
g	gas
i	species
iso	isolated
l	liquid phase
M	mass transfer
p	constant pressure
r	reference
s	surface, swelling or non-evaporating liquid
total	total
T	heat transfer
v	vapour phase
0	value at the beginning of a time step or initial value
1	value at the end of a time step
∞	ambient

Superscripts

sat	saturated
—	average

evaporating liquid, or a non-evaporating substance dissolved in this liquid. This process eventually leads to the formation of a solid (dry) residue, and the process itself is called drying. As mentioned in the previous section, small solid particles dispersed in an ambient evaporating liquid, or a non-evaporating substance dissolved in this liquid, can be treated as non-evaporating components. This allows us to treat drying droplets as at least bi-component. The droplets are assumed to be perfectly spherical. Three key sub-processes involved in the process of droplet drying will be considered separately in the following sub-sections: droplet heating/cooling, diffusion of the components inside droplets, and evaporation of the volatile component.

2.1. Droplet heating/cooling

The process of droplet heating/cooling is described by the transient heat conduction equation for the temperature $T \equiv T(t,R)$ in the liquid phase, assuming that all processes are spherically symmetric [22,23]. An analytical solution to this equation, subject to the initial, $T(t=0) = T_{d0}(R)$, and boundary condition (assuming that the effects of evaporation can be ignored),

$$h(T_g - T_s) = k_{\text{eff}} \frac{\partial T}{\partial R}\bigg|_{R=R_d-0}, \tag{1}$$

and assuming that the convection heat transfer coefficient $h = \text{const}$, can be presented as [24]:

$$T(R,t) = \frac{1}{R}\sum_{n=1}^{\infty}\left\{ q_n \exp\left[-\kappa_R\lambda_n^2 t\right] - \frac{R_d^2 \sin\lambda_n}{||v_n||^2\lambda_n^2}\mu_0(0)\exp\left[-\kappa_R\lambda_n^2 t\right] - \frac{R_d^2\sin\lambda_n}{||v_n||^2\lambda_n^2}\int_0^t \frac{d\mu_0(\tau)}{d\tau}\exp\left[-\kappa_R\lambda_n^2(t-\tau)\right]d\tau\right\} \times \sin\left[\lambda_n\left(\frac{R}{R_d}\right)\right] + T_g(t), \tag{2}$$

where λ_n are solutions to the equation:

$$\lambda\cos\lambda + h_0\sin\lambda = 0, \tag{3}$$

$$||v_n||^2 = \frac{R_d}{2}\left(1 - \frac{\sin 2\lambda_n}{2\lambda_n}\right) = \frac{R_d}{2}\left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right),$$

$$q_n = \frac{1}{||v_n||^2}\int_0^{R_d}\widetilde{T}_0(R)\sin\left[\lambda_n\left(\frac{R}{R_d}\right)\right]dR, \quad \kappa_R = \frac{k_{\text{eff}}}{c_l\rho_l R_d^2},$$

$$\mu_0(t) = \frac{hT_g(t)R_d}{k_{\text{eff}}},$$

$h_0 = (hR_d/k_{\text{eff}}) - 1$, $\widetilde{T}_0(R) = RT_{d0}(R)$. The solution to Eq. (3) gives a set of positive eigenvalues λ_n numbered in ascending order