New approaches to hydrodynamic modelling of heating and evaporation of droplets and liquid films

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Abstract

Some of the most recent developments in the modelling of droplet and liquid film heating and evaporation, published in the *International Journal of Heat and Mass Transfer* in 2018-2019, are reviewed. These developments are focused on droplet drying with a pharmaceutical application, liquid film heating and evaporation with automotive applications, and micro-explosions in water-fuel emulsion droplets with automotive applications. The new model for drying of spherical droplets is based on the analytical solutions to the species diffusion and heat transfer equations inside droplets. Solid particles, or a non-evaporating substance dissolved in the liquid, are treated as a non-evaporating component. The model was used to analyse the spray of chitosan dissolved in water. The predicted size of the residual solid balls was shown to be consistent with that observed experimentally. The new model for multi-component liquid film heating and evaporation is based on the analytical solutions to the species diffusion and heat transfer equations inside the film. The Robin boundary condition at the film surface, and the Dirichlet boundary condition at the wall, were used for the solution to the heat transfer equation. The Neumann boundary conditions at the wall, and Robin boundary conditions at the film surface, were used to solve the species diffusion equation. The constant convective heat transfer coefficient was assumed. The convective mass transfer coefficient was estimated from the Chilton-Colburn analogy. The model was applied to the analysis of a film composed of a 50%/50% mixture of heptane/hexadecane in Diesel engine conditions. The new model for the puffing/micro-explosion of water-fuel emulsion droplets is based on the assumption that a small spherical water sub-droplet is located in the centre of a fuel (n-dodecane) droplet. The heat conduction equation is solved inside this droplet using the Dirichlet boundary condition at its surface. It is assumed that the puffing/micro-explosion process starts when the temperature between water and fuel reaches the boiling temperature of water. The model predictions are shown to be consistent with available experimental data referring to the time to puffing/micro-explosion.

Keywords

Droplets, Film, Heating/evaporation, Drying, Micro-explosions.

Introduction

The modelling of droplet and liquid film heating and evaporation has long attracted the attention of researchers in various fields of engineering, pharmaceuticals and environmental science [1]. A detailed review of various models of these processes, referring mainly to droplets in automotive applications, was presented by one of co-authors in his recent monograph and review paper [2, 3].

The current review describes new models of droplet and liquid film heating and evaporation which were not considered in [2, 3]. These models focus on droplet drying, multi-component liquid film heating and evaporation and puffing/micro-explosion in water-fuel emulsion droplets. Although these models are described in three papers recently published in the *International Journal of Heat and Mass Transfer* [4, 5, 6], they have never been reported to the ILASS community. This is the rationale behind the preparation of this paper and presentation of the results at the ILASS conference.

The main ideas of these models and some results of their application to pharmaceutical and engineering problems are described in the following three sections.

Drying of droplets

The model for droplet drying, described in [4], focuses on the analysis of heating and evaporation of droplets containing solid particles dispersed in an ambient volatile liquid, or a non-evaporating substance dissolved in this liquid. This process produces a solid residue (drying). Solid particles or a non-evaporating substance were treated as non-evaporating components. This makes it possible to treat drying droplets as bi-component droplets. Droplets were assumed to be perfectly spherical. Three sub-processes involved in the process of droplet drying within this model were taken into account: droplet heating or cooling; diffusion of the droplet components; and evaporation of the droplet's volatile component from the droplet surface.

The heat transfer and species diffusion inside droplets were considered based on the analytical solutions to heat transfer and species diffusion equations with Robin boundary conditions at the surfaces of the droplets. These solutions were presented and described in [2, 3]. The ambient liquid was assumed to be ideal and Raoult's law was used. The Abramzon and Sirignano model (see [2] for the details) was used for the analysis of the processes in the gas phase and thermal swelling of droplets was taken into account.
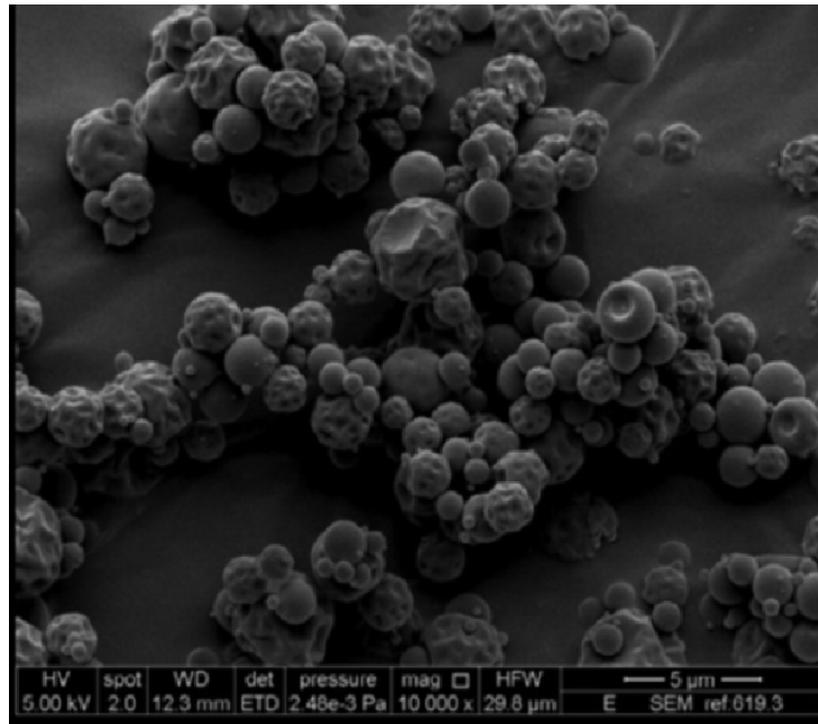
Figure 1. A typical scanning electron microscopy micrograph for chitosan particles after spray drying. Reprinted from International Journal of Heat and Mass Transfer, Volume 122, Sazhin et al., A new model for a drying droplet, Pages 451-458, Copyright Elsevier (2018).

The model was applied to the preparation of chitosan particles by spray drying. Scanning electron microscopy was used to determine the structural characteristics, surface morphology and visual particle sizes. A typical scanning electron microscopy micrograph for the chitosan particles is shown in Figure 1.

During the drying process, droplets were created from a solution of a polymer (0.2 g) in water (50 g). This led to the initial mass fraction of 0.4% for the polymer. The drying gas had temperature 393 K and was at atmospheric pressure. The average gas velocity was estimated to be 0.00933 m/s. The initial droplet diameters and temperatures were assumed to be 20 μm and 293 K, respectively.

The plots of mass fractions of water and chitosan at the droplet surface, predicted by the model using the above-mentioned assumptions, are shown in Figure 2. As follows from Figure 2, the relative mass fraction of chitosan in the mixture is negligibly small at times less than about 0.1 s. At later times, however, the mass fractions of both substances become comparable. At times close to 0.127 s, the mass fraction of chitosan exceeds that of water.

The predicted diameters of the balls of polymer (about 3 μm), formed after the drying process has completed, are compatible with the diameters of observed particles shown in Figure 1.

Liquid film heating and evaporation

Various approaches to the modelling of multi-component liquid film heating and evaporation have been considered in many papers (see [5] for the details). The simplest is based on the assumption that liquid species and thermal diffusivities are infinitely large (zero-dimensional model). Recently, numerous approaches to taking into account their finite values, leading to the formation of gradients of species mass fractions and temperature inside the film, were suggested. We believe that the model taking into account these effects, suggested in [5], is one of the most advanced. It has proven to be useful for various applications including those of automotive engineering.

The model suggested in [5] is based on the assumption that the gradients of temperature and species mass fractions in the film perpendicular to the surface of the wall are much larger than those parallel to the surface of the wall. This allowed the authors of [5] to describe the heat transfer and species diffusion processes in the film using the one-dimensional transient diffusion equations. The Robin boundary condition at the film surface, and the Dirichlet boundary condition at the wall, were used for the solution to the heat transfer equation. The Neumann boundary conditions at the wall, and Robin boundary conditions at the film surface, were used to solve the species diffusion equation. Both equations were solved analytically, and this analytical solution was incorporated into the numerical code where it was used at the end of each time step. The convective heat transfer coefficient h was assumed to be constant while the convective mass transfer coefficient was inferred from the Chilton-Colburn analogy. The thermal swelling of the film was taken into account.

The result of the validation of the model for the evaporation of a film composed of mixtures of isooctane/3-methylpentane (3MP) is shown in Figure 3. Three cases were considered: pure isooctane, pure 3MP, and a 50%/50% mixture of isooctane and 3MP. Gas and wall temperatures were assumed to be the same and equal to 302.25 K. Initially the
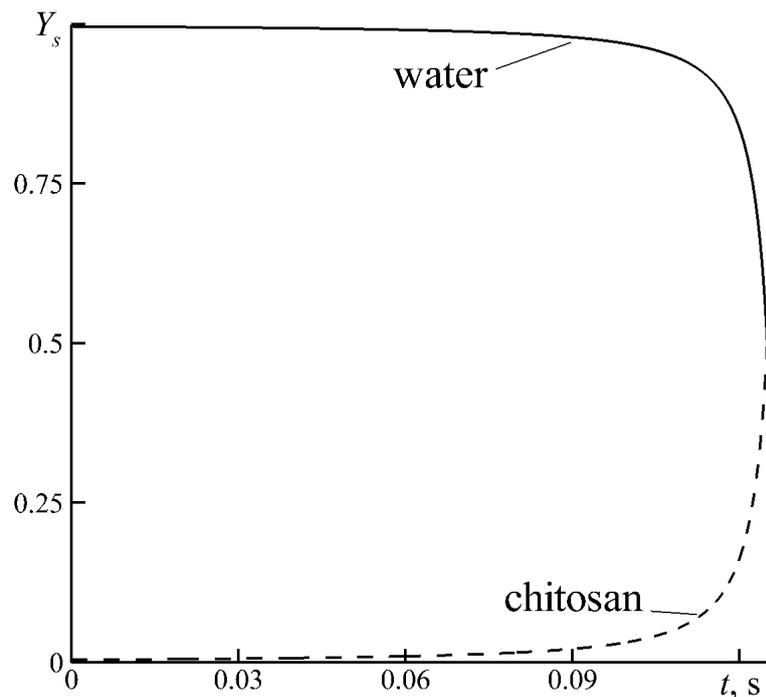
Figure 2. Chitosan and water mass fractions at the droplet surfaces versus time for input parameters described in the paper. Reprinted from International Journal of Heat and Mass Transfer, Volume 122, Sazhin et al., A new model for a drying droplet, Pages 451-458, Copyright Elsevier (2018).

temperature of liquid in the film was assumed to be homogeneous and equal to 293.15 K. The initial film thickness and the convection heat transfer coefficient were taken as 293.15 K and 14 W/(m²K), respectively.

One can clearly see from this figure that the results of calculations are close to the experimental data for all cases. This allows us to use the model to analyse other liquid films including those in automotive application.

One of these applications focused on the analysis of a liquid film composed of a 50%/50% mixture of n-heptane and n-hexadecane under Diesel engine-like conditions. It was shown that at first the film thickness decreased rapidly until all n-heptane had evaporated. Then the rate at which the film thickness decreased slowed down. The film's average temperature and surface temperature were shown to increase quickly at the initial stage of the process until these temperatures reached the maximal values. Then both temperatures decreased until they reached the wall temperature when the film completely evaporated. The predicted timescale of evaporation was shown to be consistent with the results of measurements of thin fuel films under Diesel engine conditions.

Micro-explosions

The interest in micro-explosions has been mainly stimulated by the possible contribution of this process to rapid disintegration of fuel droplets in automotive engines (secondary break-up). This disintegration enhances the fuel droplet size distribution, leads to effective air-fuel mixing, and ultimately results in better fuel efficiency. Micro-explosions are typically preceded by puffing and both these processes are usually modelled together.

The main focus of the modelling of this phenomenon has been to achieve a highly detailed description of the processes involved. Perhaps the most advanced model developed along these lines was the one suggested by Shinjo et al. [7, 8], but whilst it is expected to be very useful for understanding the processes that take place during the puffing and micro-explosion of droplets, its usefulness for investigating engineering processes is less obvious. Practitioners studying these processes are interested mainly in their integral characteristics, such as puffing/micro-explosion delay times, rather than in the fine details of the phenomena inside the droplet leading to their micro-explosion.

The model developed in [6] is focused primarily on predicting this delay time ignoring most details of the processes leading to micro-explosions. The main assumption of the model is that a spherical water sub-droplet is located in the centre of a larger fuel droplet (see Figure 4). The fuel is identified as n-dodecane, although any other hydrocarbon fuel could be used. Water sub-droplet and fuel droplet are assumed to be concentric spheres.

The droplet surface temperature was assumed constant; fuel evaporation and droplet motion were not taken into account. The droplet heating from its surface to its interior was described by a one-dimensional transient spherically symmetric heat conduction equation. The analytical solution to this equation inside the composite droplet with the Dirichlet boundary condition at its surface was found. This solution leads to a time-dependent distribution of temperature inside the droplet.

For droplet surface temperature larger than its initial inner temperature (assumed homogeneous) the temperatures inside the droplet increase. If this surface temperature is greater than the temperature of boiling water, then at some
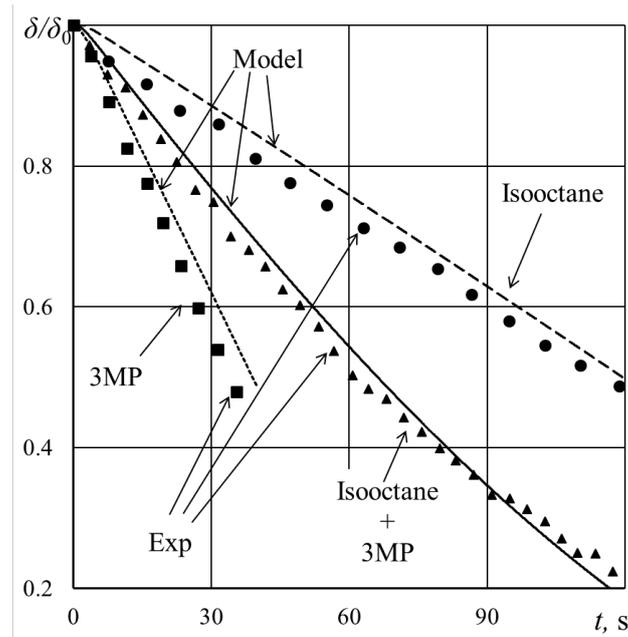
Figure 3. The normalised film thickness versus time. Circles, triangles and squares show the experimental data (see [5] for the details); solid and dashed curves show the model predictions. Three cases were considered: pure isooctane, pure 3MP, and a 50%/50% mixture of isooctane and 3MP. Reprinted from International Journal of Heat and Mass Transfer, Volume 117, Sazhin et al., A mathematical model for heating and evaporation of a multi-component liquid film, Pages 252-260, Copyright Elsevier (2018).
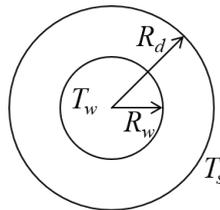
Figure 4. The location of a water sub-droplet of radius R_w inside the fuel droplet with radius R_d. The temperature at the interface between water and fuel is T_w; the droplet surface temperature is T_s. Reprinted from International Journal of Heat and Mass Transfer, Volume 131, Sazhin et al., A simple model for puffing/micro-explosions in water-fuel emulsion droplets, Pages 815-821, Copyright Elsevier (2019).

stage the temperature at the surface of the water sub-droplets reaches the boiling temperature of water. The time instant when this happens is identified as the start of the puffing/micro-explosion process. This time is called the time to puffing, or the delay time for the micro-explosion. The maximal value of the droplet surface temperature is taken equal to the n-dodecane boiling temperature. For this temperature, the delay time is anticipated to be minimal. To validate the predictions of the model, we considered typical initial values of input parameters (n-dodecane droplets with water sub-droplets, the surface temperatures of droplets and ambient gas parameters). These are shown in Table 1, where 489.47 K is the n-dodecane boiling temperature. For all these parameters the temperatures, predicted by the analytical solution, versus the normalised distance from the droplet centre (R/R_d) at various time instances were obtained. These results allowed us to identify the time instants when T_w reached the boiling temperature of water for each set of parameters shown in Table 1.

These time instances, identified as times to puffing/micro-explosion, are shown in Figure 5 as functions of diameters of droplets for the initial and surface temperatures of droplets presented in Table 1. The times to puffing/micro-explosion, observed experimentally for various droplet diameters, are presented in the same figure.

As follows from Figure 5, the predicted times to puffing/micro-explosion when droplet surface temperature equalled the n-dodecane boiling temperature were always less than those observed experimentally. In most cases, the magnitudes of the predicted times to puffing/micro-explosion for other values of the surface temperature of droplets turned out to be of the same order of magnitude as observed experimentally. Hence, the new model is able to describe the underlying processes leading to puffing/micro-explosion qualitatively and in some cases even quantitatively. This happens despite the obvious simplicity of this model.

Conclusions

An overview of some recent developments in the modelling of droplet and liquid film heating and evaporation is presented. These developments refer to droplet drying, liquid film heating and evaporation, and micro-explosions in water-fuel emulsion droplets. The new model for drying of spherical droplets is based on the analytical solutions
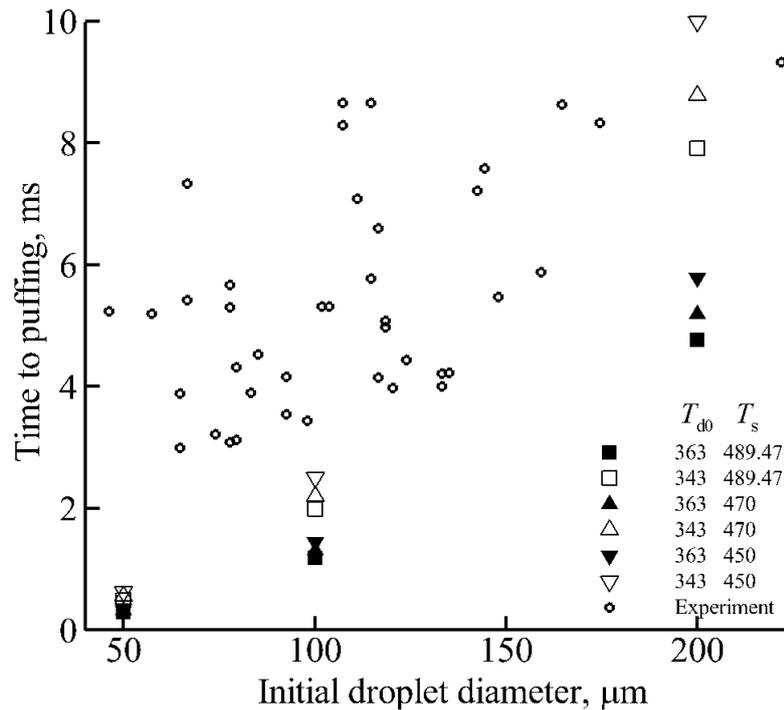
Figure 5. The values of time to puffing/micro-explosion, predicted by the model, versus the initial droplet diameters for 2 values of the initial droplet temperature and 3 values of droplet surface temperature (see the insert). The experimentally observed values of this time are shown as empty circles. Reprinted from International Journal of Heat and Mass Transfer, Volume 131, Sazhin et al., A simple model for puffing/micro-explosions in water-fuel emulsion droplets, Pages 815-821, Copyright Elsevier (2019).

Table 1. The properties of droplets and gas used for the validation of the model.

Parameter	Values
Parent droplet radii (R_d) [μm]	25; 50; 100
Droplet initial composition [vol]	0.15 water + 0.85 n-dodecane
n-dodecane density (ρ_f) [kg/m^3]	25; 50; 100
Gas composition	air
Droplet surface temperatures (T_s) [K]	489.47; 470; 450
Initial droplet temperature (T_{d0}) [K]	343; 363
Gas (air) pressure [MPa]	0.1

to the species diffusion and heat transfer equations inside droplets. Solid particles, or a non-evaporating substance dissolved in the liquid, are treated in this model as non-evaporating components. The model has been used to analyse the spray of chitosan dissolved in water. The predicted sizes of the residual solid balls were shown to be consistent with those observed experimentally.

The new model for multi-component liquid film heating and evaporation, based on the analytical solutions to the species diffusion and heat transfer equations inside the film, is reviewed. The Robin boundary condition at the film surface, and the Dirichlet boundary at the wall, are used for the solution to the heat transfer equation. The Neumann boundary conditions at the wall, and Robin boundary conditions at the film surface, are used to solve the species diffusion equation. The convective heat transfer coefficient is assumed to be constant. The convective mass transfer coefficient is estimated from the Chilton-Colburn analogy. The model was applied to the analysis of a film composed of a 50%/50% mixture of heptane/hexadecane in Diesel engine-like conditions.

Finally, the new model for the puffing/micro-explosion of water-fuel emulsion droplets is reviewed. This model is based on the assumption that a small spherical water sub-droplet is located in the centre of a fuel (n-dodecane) droplet. The heat conduction equation is solved inside this droplet using the Dirichlet boundary condition at its surface. It is assumed that the puffing/micro-explosion process starts when the temperature at the interface between water and fuel reaches the boiling temperature of water. The model predictions are consistent with available experimental data referring to the time to puffing/micro-explosion.

Nomenclature

R	distance from the droplet centre [m]
R_d	droplet radius [m]
t	time [s]
T	temperature [K]
Y	mass fraction [-]
ρ	density [kg/m^3]

Subscripts

b	boiling
d	droplet
f	fuel
s	surface
w	wall or the surface of a water sub-droplet
0	initial

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