Effect of local surface curvature on heating and evaporation of deformed droplets

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Introduction

Drop evaporation in gaseous flows is of fundamental importance for a wide range of engineering applications (automotive, aeronautic, fire suppression, painting, medical aerosol, meteorology, etc.). This process involves simultaneous heat and mass transfer and a wide literature is available on the modelling of the complex physical phenomena involved (see [1] for a recent review on the subject). Liquid droplets interacting with the carrier gas phase are subject to deformation, due to the interaction of surface tension and fluid-dynamic stresses on the drop surface. While surface tension force induces a spherical shape, fluid-dynamic forces are the primary sources of drop deformation. This is clearly evident in case of liquid drop with Weber number above 2, typical of spray combustion applications, which are appreciably non-spherical. The simplifying hypothesis of drop sphericity, which is the basis of all the models currently implemented in CFD codes for spray analysis [2], can only be considered as an idealisation. Recently [3], this hypothesis was removed, developing analytical solutions to the problem of heating and evaporation from spheroidal and triaxial ellipsoidal drops. The present investigation aims to extend the previous work, proposing a model based on the analytical solution of the species and energy conservation equations within the gas phase surrounding a single-component deformed drop and to analyse the effect of local curvature on the local evaporation and heat fluxes for a wider range of drop shapes.

Mathematical modelling

The species conservation equations for a single component drop evaporating under quasi-steady conditions are:

$$\nabla_j N_j^{(p)} = 0 \qquad p = (0,1) \tag{1}$$

where:

$$N_j^{(p)} = N_j^{(T)} y^{(p)} - cD_{10} \nabla_j y^{(p)} \tag{2}$$

are the molar fluxes, p=1 stands for the evaporating species while p=0 for the non-evaporating one, $N_j^{(T)} = N_j^{(0)} + N_j^{(1)}$ and $y^{(p)}$ is the molar fraction of the species p and c is the molar gas density that, under the assumption of ideal gas mixture, can be calculated as:

$$c = \frac{P_T}{RT} \tag{3}$$

To notice that the usual way to approach this problem is by using a mass form of the species conservation equations (see [2]), but it can be shown (see [4]) that for single component drops the two approaches are equivalent and the mass flux can be obtained by $n_j^{(p)} = N_j^{(p)} Mm^{(p)}$.

Assuming that the non-evaporating component p=0 does not diffuse into the liquid and considering that, for the quasi-steady approach, the drop surface is assumed to be still, the molar flux of this species is nil everywhere and:

$$N_j^{(1)} = N_j^T = cD_{10} \nabla_j H \tag{4}$$

where $H = \ln\left(y^{(0)}\right)$. Summation of equations (1) yields the mass conservation equation:

$$\nabla_j \left(\rho U_j\right) = 0 \tag{5}$$

and, since under the mentioned assumptions: $\rho U_j = n_j^{(T)} = n_j^{(1)} = Mm^{(1)} N_j^{(T)}$, equations (4) and (5) yield:

$$\nabla^2 H = 0 \tag{6}$$

The steady energy equation, assuming constancy of the thermo-physical properties, using equations (5) and neglecting some minor terms (see [5] for a more detailed discussion), becomes:

$$\nabla_j H \nabla_j T - Le_M \nabla^2 T = 0 \tag{7}$$

where the modified Lewis number is defined as: $Le_M = k \big/ \left(M m^{(1)} c D_{10} c_p \right)$.

1.1. Coordinate systems and solutions

Equations (6) and (7) must be solved imposing boundary conditions at the drop surface and at infinity. For the present analysis the condition on the drop surface and at infinity will be assumed of Dirichlet type and uniform, i.e.:

$$\begin{aligned} &T(\zeta = \zeta_0) = T_s; \;\; T(\zeta = \infty) = T_\infty \\ &y^{(1)}(\zeta = \zeta_0) = y_{sat}(T_s); \;\; y^{(1)}(\zeta = \infty) = y_\infty^{(1)} \end{aligned} \tag{8}$$

The problem set by equations (6), (7) and (8) is clearly independent of the choice of the coordinate system and holds for any shape of the evaporating drop. However, proper choices of coordinate systems allow simpler solutions for a variety of drop shape. In the present work five curvilinear orthogonal coordinate systems are considered: spherical, prolate and oblate spheroidal, inverse prolate and oblate rotation cyclide, which are defined as follows [6]:

$$\begin{aligned} x &= a \frac{\sqrt{\zeta^2 + \alpha}}{\Theta} \sqrt{1-\eta^2} \cos\varphi = \Phi(\zeta,\eta)\cos\varphi \\ y &= a \frac{\sqrt{\zeta^2 + \alpha}}{\Theta} \sqrt{1-\eta^2} \sin\varphi = \Phi(\zeta,\eta)\sin\varphi \\ z &= a \frac{\zeta\eta}{\Theta} = \Psi(\zeta,\eta) \end{aligned} \tag{9}$$

where the values of α and Θ are given in table 1 for the selected coordinate systems.

Table 1. Parameters of the selected coordinate systems [6].

Shape	α	Θ		$J_n(\zeta)$
Sphere	0	1	$0 \le \zeta < 1$	$\zeta^{(n+1)}$
Oblate	+1	1	$0 \le \zeta < \infty$	$Q_n(i\zeta)$
Prolate	-1	1	$1 \le \zeta < \infty$	$Q_n(\zeta)$
Inverse oblate	+1	$\zeta^2+\alpha(1-\eta^2)$	$0 \le \zeta < \infty$	$P_n(i\zeta)$
Inverse prolate	-1	$\zeta^2+\alpha(1-\eta^2)$	$1 \le \zeta < \infty$	$Q_n(\zeta)$

The drop surface is always defined by the equation $\zeta = \zeta_0$, although it must be noticed that the coordinates η and ζ have different definitions in the different coordinate systems, as an example, $\zeta = R_0/r$ and $\eta = \cos\theta$ for the spherical coordinates, where R_0 is the radius of the spherical particle defined by the equation $\zeta = 1$ (i.e. $\zeta_0 = 1$). To notice that for a general shaped drop, an equivalent radius can be always defined as: $R_0 = \sqrt[3]{3V/4\pi}$, where V is the drop volume. In the following, the drop surface will be always defined to maintain the same equivalent radius to allow a direct comparison of the evaporation characteristics of different shaped drops having the same volume.

Spheroidal drops appear when drop oscillation is considered. The oscillation mode n=2, which is the long lasting one since viscous damping is more intense for the higher modes, it is in fact characterized by an oblate-prolate shape alternation. Drops of different shapes can be found in other kind of process, for example the head on impact of two drops at low velocity shows shapes that can be well approximated by rotational cyclides, as reported for example, in [7]. These shapes can be easily approximated in inverse oblate and inverse prolate coordinates [6].

The solutions of equations (6) and (7) assume the following forms:

$$H = \Theta^{1/2} g_0 \frac{J_0(\zeta)}{J_0(\zeta_0)} + \Theta^{1/2} \sum_{n=1}^{\infty} g_n \frac{J_n(\zeta)}{J_n(\zeta_0)} P_n(\eta) + H_\infty \tag{10}$$

$$T = \frac{e^{(H_s - H_\infty)/Le_M} T_\infty - T_s}{e^{(H_s - H_\infty)/Le_M} - 1} + \frac{T_s - T_\infty}{e^{(H_s - H_\infty)/Le_M} - 1} e^{(H - H_\infty)/Le_M} \tag{11}$$

where the function J_n are defined in table 1 for the different coordinate systems.

The normal component of the sensible heat flux at drop surface is:

$$\varphi_{\zeta} = -k \frac{1}{h_{\zeta}} \left(\frac{\partial T}{\partial \zeta} \right)_{\zeta 0} \tag{12}$$

where h_{ζ} is the proper scale factor.

2. Mass fluxes and surface curvatures

The vapour fluxes at drop surface can be found, from their definitions (4), once the function H is calculated. The available results on evaporation from non-spherical drops have considered that a direct relation between flux and surface curvature should exist. For example [8] assumed a proportionality between the vapour fluxes at drop surface and the mean curvature. Recently [3], it has been proven that for spheroidal drops there exist a perfect proportionality of the vapour flux with the fourth root of the Gaussian curvature. However, for a general drop shape the one-to-one relationship between vapour flux and local curvature has been only conjectured. The results of this investigation prove that such a conjecture cannot be supported by theory.

The principal curvatures of a generic rotational surface defined parametrically as:

$$x = \Lambda(\zeta_0, \eta) \cos\varphi; \;\; y = \Lambda(\zeta_0, \eta) \sin\varphi; \;\; z = \Psi(\zeta_0, \eta) \tag{13}$$

can be calculated as:

$$k_1 = \frac{-sign(\Lambda)\left[\Lambda_{\eta\eta}\Psi_{\eta} - \Lambda_{\eta}\Psi_{\eta\eta} \right]}{\left(\Lambda_{\eta}^2 + \Psi_{\eta}^2 \right)^{3/2}}; \quad k_2 = \frac{\Psi_{\eta}}{|\Lambda| \left(\Lambda_{\eta}^2 + \Psi_{\eta}^2 \right)^{1/2}} \tag{14}$$

and the corresponding Gaussian and mean curvatures are defined as:

$$\bar{K}_G = k_1 \, k_2; \quad \bar{C}_m = k_1 + k_2 \tag{15}$$

respectively. To generalize the analysis, considering that the drop size is always defined by the equivalent radius, the non-dimensional Gauss and mean curvature are defined as:

$$K_G = R_0^2 \bar{K}_G; \quad C_m = R_0 \bar{C}_m \tag{16}$$

In the next session the relationship between these curvatures and the corresponding non-dimensional vapour fluxes:

$$n_{\zeta,ad} = \frac{n_{\zeta}^{(1)} R_0}{\rho D_{10} \left(H_{\infty} - H_s \right)} \tag{17}$$

which are independent of the species properties, will be analysed.

3. Curvature map and vapour fluxes

From equations (16) the Gauss and mean non-dimensional curvatures can be calculated for the above reported drop shapes. Figure 1(a) shows a sample of the contour distribution of the two non-dimensional curvatures for two rotational cyclides (inverse oblate and inverse prolate), while figure 1(b) shows the corresponding 2D map for all the selected drop shapes. Different shapes are characterised by different non-dimensional local curvatures as a function of shape (i.e. ζ_0) and position on the surface (i.e. η), and the map shows that there exists a relatively narrow region where four drop shapes, namely oblate and prolate spheroids, inverse prolate and oblate cyclides, have the same Gauss and mean curvature in some positions over the drop surface.

Since the curvature characteristics of a surface are completely defined by these two curvatures, the existence of a direct relationship between surface curvature and vapour flux would imply that the four drops have the same vapour fluxes at the locations where the curvatures are the same.

Figure 2 reports the map of the non-dimensional vapour flux for the four surfaces, calculated into the above mentioned overlapping region. The shape of the map for the oblate/prolate spheroids confirms the known direct dependence to the fourth root of the Gaussian curvature, a results that was established not only for spheroidal shapes but also for triaxial ellipsoids (see [3]). However, the map for the other two drop shapes shows a quite different dependence.

This proves that the vapour flux from a deformed drop cannot in general be only a function of local curvature. This does not disprove the above mentioned results for ellipsoidal drops, in the sense that it is possible, as above stated, that for a certain class of shapes a relationship exists, but this cannot be considered a general rule.

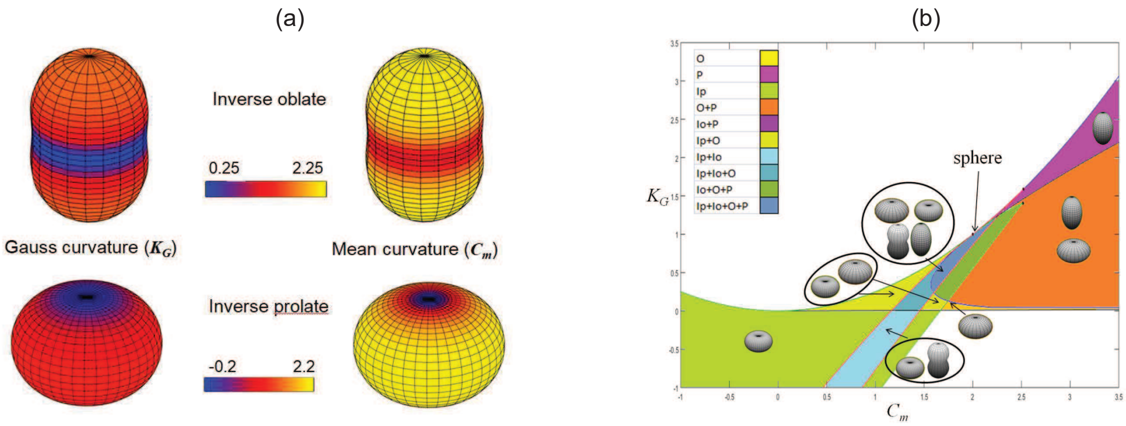

Figure 1. (a) Samples of contour distributions of Gauss and mean curvatures for two rotational cyclides; (b) map of Gauss and mean surface curvatures for different drop shapes.

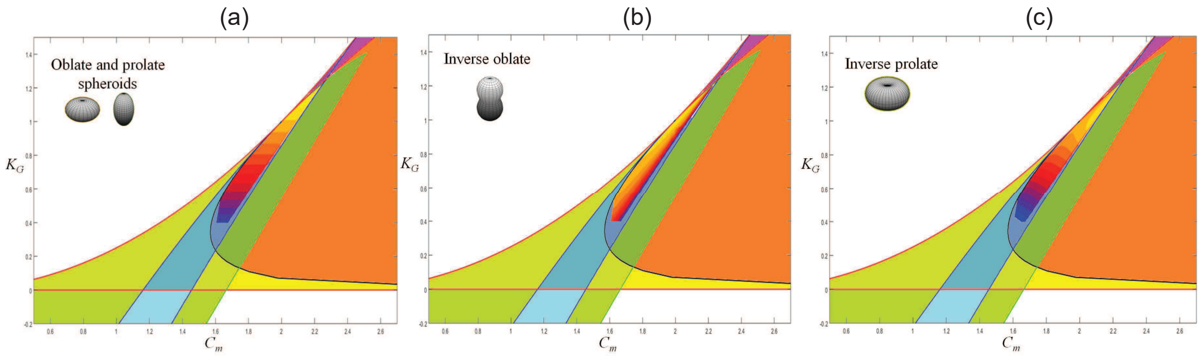

Figure 2. Map of the non-dimensional vapour fluxes for (a) the oblate and prolate spheroids, (b) the inverse oblate and (c) inverse prolate cyclides, calculated into the overlapping region.

4. Conclusions

An analytical model has been developed to calculate the drop evaporation accounting for the effect of drop deformation. The model is applied to five drop shapes, namely the sphere, the oblate and prolate spheroids, and two rotation cyclides (inverse oblate and prolate spheroids). Some common simplifying hypotheses, like steady-state, constant gas properties, single component drop, are assumed. The conservation equations are solved in each natural coordinate system, depending on the drop shape, imposing uniform Dirichelet boundary conditions at the drop surface and at free-stream. The local vapour flux over the drop surface is calculated and correlated, where possible, with the local curvature. It is confirmed that for spherical and spheroidal drops the local vapour flux is proportional to the fourth root of the surface Gaussian curvature, and this result can be also extended to triaxial ellipsoidal drops, while for inverse spheroidal drops the local fluxes depend both on the local curvature and the whole drop shape.

This proves that the local vapour flux from a deformed drop cannot in general be only a function of local curvature, although this can happen for certain classes of drop shapes (like for ellipsoidal drops).

References

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