OSCILLATING DROPLET EVAPORATION MODELLING FOR SPRAY COMBUSTION SIMULATION

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ABSTRACT
The vapour and gas phase conservation equations are analytically solved in a spheroidal coordinate systems, yielding the drop surface vapour flux under steady-state conditions, for oblate and prolate drops. The drop evaporation rate can be defined as function of drop spheroid shape and drop surface. The solution is easily implementable to the case of prolate/oblate oscillating drops, under quasi-steady assumption, which is found to be valid under the range of operating conditions typical of spray combustion applications.

INTRODUCTION

The majority of liquid spray numerical models requires information on the behaviour of an individual liquid drop in a gaseous flow [1]. Simplified models for predicting the drop phenomena in a spray (aerodynamic forces, evaporation, collision, break-up) have been developed through analytic, experimental, and numerical studies of individual liquid drops. These models usually assume a spherical shape for the liquid drop; for example the modelling of drop evaporation in most commercial CFD code for spray numerical simulations is generally based on this assumption [2]. On the other hand, a spray consists of liquid drops that undergo significant shape deformations while interacting with the carrier phase [3]. More generally, dispersed fluid particles (bubbles and drops, away from walls) can deform based on the interaction of surface tension and the fluid-dynamic stresses on the particle surface [4]. The surface tension forces will always drive a free particle towards a spherical shape, whereas initial conditions and/or fluid-dynamic forces are the primary sources of non-sphericity.

Examining the deformation response, three competing effects are found responsible of drop deformation [1]. The first one is a convective effect in the gas phase which tends to generate oblate drops. The second one is a convective effect in the liquid phase, which induces the deformation towards the prolate shape. The third one is a combined effect of gas-phase viscous and convective forces; this is considered important in large Ohnesorge number cases and tends to cause dimpled shapes [1].

The drop deformation could have significant effects on inter-phase transfer phenomenon, thus resulting in some modifications in the existing correlations valid for spherical drops [3]. The numerical treatment of this effect should take into account the continuously evolving interface that is very closely coupled to the heat and mass transfer occurring in the drop. Previous studies concluded that the dynamics of the drop deformation is basically unaffected by vaporization, however, the evaporation rates (per unit area) are greater for deformed drops [5].

Several studies available in the literature found that heat and mass transfer between liquid particles and the surrounding gas can be enhanced by drop oscillations [6, 7]. Particle oscillation can be achieved by a variety of methods, including acoustic oscillation, electric field oscillation for charged particles, and magnetic field oscillation for magnetic particles [6].

Furthermore, drop-gas interaction activates many drop oscillation modes and actually no drop in a gaseous stream can be steadily spherical. Haywood et al. [8] show that circulation inside the drop is responsible for the strong damping and promotes the formation of prolate shapes for drops. They also found that effect of liquid viscosity and finite amplitude oscillation reduces the drop oscillation frequencies up to 25% of the theoretical natural frequency predicted by Lamb [9]. Moreover, the results from [3] show that the mass flux varies along the surface of the deformed drop, due to modifications of the isotherms near the interface.

Drop oscillations can become important in atomization systems, where the liquid is first disintegrated into small ligaments, which then oscillate towards the attainment of an equilibrium spherical shape. If these ligaments/drops are exposed to a hot gas then the heat and mass transfer could be affected by oscillations. The rate of evaporation of an oscillating drop varies in time, but it is always greater than or equal to the rate of evaporation of the equivalent spherical drop [5].

Mashayek [3] suggested a correction in the evaporation rate of a deformed drop, derived from the results obtained by numerical simulations. The model, valid for surface deformation up to 10% of the drop radius, predicts that the rate of evaporation increases with the increase of the amplitude of the surface deformation and varies significantly along the surface of the drop. The same author in [10] proposed an application of the correction to the case of free oscillating drops, showing that the increase in the evaporation rate results to be proportional to the square of the surface disturbance amplitude and larger for higher oscillating modes [10].

Since the early work of Lamb [8], drop oscillation was the subject of many investigations, and the open literature is rich of works on this important phenomenon. Linear theory was widely used to obtain results for small amplitude oscillation, perturbation theory and non-linear analysis were used to extend the results to moderate and large amplitude oscillation and effect of viscosity was shown to quickly damp the highest modes, then living only the oblate-prolate mode to survive and, among many other results, it was observed that drops, which are released from an initially

two-lobed configuration spend less time in prolate form than in oblate one [11].

The necessity to include such complex behaviour in spray numerical simulations, prompts the continuous request of relatively simple sub-models for predicting the inter-phase phenomena taking place during the spray evolution. The present work proposes a rather easy-to-implement analytical expression of the instantaneous evaporation rate from oblate and prolate spheroid liquid drops and a possible application to the calculation of evaporation enhancement in oscillating drops. The derivation of the mathematical model is briefly presented in the following section, followed by the description of the model application to oscillating drops. Finally the main conclusions are briefly summarised.

MATHEMATICAL MODEL

Specie transport equations

For a liquid drop made of a single component floating in a gaseous atmosphere, the specie conservation equations can be written as [12]:

$$\rho U_j \nabla_j \chi_\alpha = \nabla_j \left(\rho D_v \nabla_j \chi_\alpha \right) \tag{1}$$

where $\alpha = v, g$ refers to the vapour and gaseous phases respectively, while $\chi_\alpha = \dfrac{\rho_\alpha}{\rho}$ is the mass fraction.

The boundary conditions (B.C.) set to constant values the vapour mass fraction at drop surface $\left(\chi_{v,s} \right)$ and at infinite distance from the drop $\left(\chi_{v,\infty} \right)$.

Integrating equations (1), the specie fluxes are calculated as:

$$\gamma_\alpha = \rho U_j \chi_\alpha - \rho D_v \nabla_j \chi_\alpha \tag{2}$$

with the first term representing the Stefan flow component [12] and the second being the diffusive component.

Evaporation rate of spheroid drop

To find an analytical solution for spheroidal drops, equation (1) must be written in a proper system of coordinates, and the natural choice are spheroidal coordinates, that for the oblate and prolate cases are defined as follows:

Oblate	Prolate
$x = a \cosh \xi \sin \theta \cos \varphi$	$x = a \sinh \xi \sin \theta \cos \varphi$
$y = a \cosh \xi \sin \theta \sin \varphi$	$y = a \sinh \xi \sin \theta \sin \varphi$
$z = a \sinh \xi \cos \theta$	$z = a \cosh \xi \cos \theta$

In these coordinate systems, the spheroid surface equation is simply $\xi = \xi_0$ and the B.C. are then:

$$\chi_v \left(\xi_0, \theta, \varphi \right) = \chi_{v,s} \qquad \chi_v \left(\infty, \theta, \varphi \right) = \chi_{v,\infty} \tag{3}$$

A steady state analytical solution of the balance equations (1) and B.C. (3) exists under the form:

Oblate: $\chi_v = 1 - \left(1 - \chi_{v,s} \right) \left(\dfrac{1 - \chi_{v,\infty}}{1 - \chi_{v,s}} \right)^{\frac{\arctan\left(e^\xi\right) - \arctan\left(e^{\xi_0}\right)}{\frac{\pi}{2} - \arctan\left(e^{\xi_0}\right)}}$

Prolate: $\chi_v = 1 - \left(1 - \chi_{v,s} \right) \left(\dfrac{1 - \chi_{v,\infty}}{1 - \chi_{v,s}} \right)^{1 - \frac{\ln\left(e^\xi + 1\right) - \ln\left(e^\xi - 1\right)}{\ln\left(e^{\xi_0} + 1\right) - \ln\left(e^{\xi_0} - 1\right)}}$

From these solutions, the evaporation rate can be easily calculated by integrating equation (2) over the drop surface, yielding, in non-dimensional form:

$$\hat{m}_{ev} = \frac{m_{ev}}{4 \pi R_0 \rho D_v} = C(\varepsilon) \ln \frac{1 - \chi_{v,\infty}}{1 - \chi_{v,s}} \tag{4}$$

where the parameter ε is defined as:

$$\varepsilon = \frac{a_z}{a_r}$$

and a_z and a_r are respectively the axial and radial spheroid axes, see Figure 1 for reference.
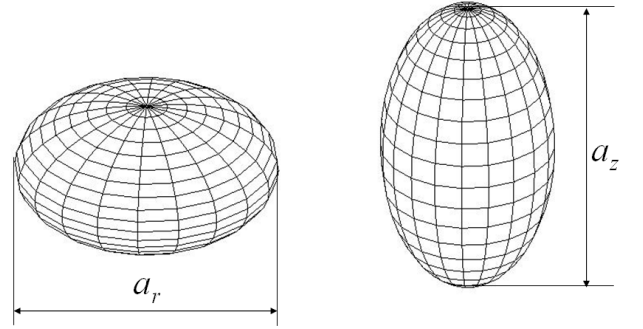

Figure 1. Oblate (left) and prolate (right) spheroids and definition of axial (a_z) and radial (a_r) spheroid axes.

The parameter $C(\varepsilon)$ in equation (4) is defined as follows:

$$C(\varepsilon) = \begin{cases} \dfrac{\sqrt{1 - \varepsilon^2}}{\varepsilon^{1/3} \left(\pi - 2 \arctan \sqrt{\dfrac{1 + \varepsilon}{1 - \varepsilon}} \right)} & , \varepsilon < 1, \text{ Oblate} \\[20pt] \dfrac{\sqrt{\varepsilon^2 - 1}}{\varepsilon^{1/3} \left[\ln \left(\sqrt{\dfrac{\varepsilon + 1}{\varepsilon - 1}} + 1 \right) - \ln \left(\sqrt{\dfrac{\varepsilon + 1}{\varepsilon - 1}} - 1 \right) \right]} & , \varepsilon > 1, \text{ Prolate} \end{cases}$$

and $C = 1$ for a sphere $\left(\varepsilon = 1 \right)$.

It is of a certain interest to evaluate the surface of a spheroid having the same volume of a sphere with radius R_0. Defining with β the ratio between the spheroid surface and the surface of an isovolumic sphere, it is easy to show that a one-to-one relation exists between the parameters ε and β:

$$\beta(\varepsilon) = \frac{A_{spheroid}}{A_{sphere}} = \frac{1}{2 \varepsilon^{2/3}} \begin{cases} 1 + \dfrac{\varepsilon^2 \ln \dfrac{1 + \sqrt{1 - \varepsilon^2}}{\varepsilon}}{\sqrt{1 - \varepsilon^2}} & \text{Oblate} \\[20pt] 1 + \dfrac{\varepsilon^2 \arctan \sqrt{\varepsilon^2 - 1}}{\sqrt{\varepsilon^2 - 1}} & \text{Prolate} \end{cases}$$

The factor $C(\varepsilon)$ can then be related to the spheroid surface as in Figure 2. As expected, the evaporation rate of a spheroid is always larger than that of a sphere having the same volume, although that of a prolate spheroid is always

larger than that of an oblate spheroid having both the same volume and the same surface.
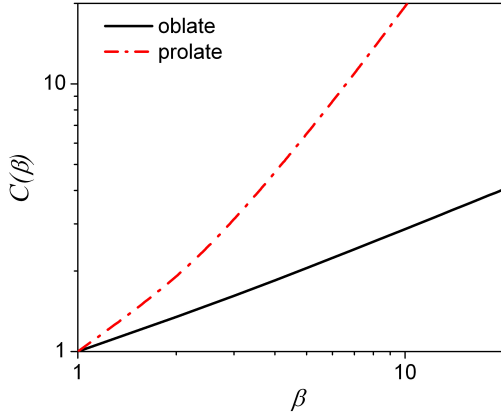

Figure 2: Non-dimensional evaporation factor as function of the spheroid surface ratio.

Oscillating drop

The oscillation modes of a liquid drop in gaseous environment can be described (for small oscillation amplitude) by the generalized Lamb equation [9].

$$\omega_n^2 = \frac{n(n+1)(n-1)(n+2)}{(n+1)\rho_{in} + n\rho_{out}} \frac{\sigma}{R_0^3} \tag{5}$$

where ρ_{in} and ρ_{out} refer to the densities of the inner and outer fluids respectively, and the index n refers to the various oscillation modes: $n=0$ stands for a pure expansion (typical for bubbles), $n=1$ refers to translation mode, without a corresponding frequency, $n=2$ refers to oblate-prolate mode, and finally $n>2$ describes more complex modes. It should be noticed that the linear theory predicts for the mode $n=2$ a shape that is only approximately oblate or prolate spheroid, although the difference for small oscillation amplitude (i.e. for the range where the linear theory holds) is almost negligible.

For a liquid drop oscillating in a gaseous environment $\rho_{in} \gg \rho_{out}$, then the Lamb equation (3) yields:

$$\omega_n^2 = \frac{n(n+1)(n-1)\sigma}{\rho_l R_0^3}$$

Considering the effect of liquid viscosity, according to [2], the higher modes are quickly damped and the mode $n=2$ is the only long lasting ones. The oscillation frequency then becomes:

$$\omega_n = \sqrt{\frac{8\sigma}{\rho_l R_0^3}}$$

As above mentioned, non linear theory [11] yields more accurate (but more complex) results, among others the fact that the time spent by a drop in the oblate shape is larger than the time spent in a prolate form, but this fact will not be considered here.

The drop shape variation of an axis-symmetric oscillating drop can be expressed through a perturbation parameter $a_n(t) = a_n^0 e^{i\varpi_n t}$ by the equation [13]:

$$r(\theta) = r_0^* \left(1 + \sum_{n=2} \frac{a_n(t)}{2n+1} P_n(\cos\theta) \right)$$

where $P_n(x)$ are the Legendre polynomials. The drop surface can then be calculated as a function of this parameter and to the third order in a_n it assumes the following expression [13]:

$$A_{spheroid} = 4\pi R_0^2 \left(\begin{array}{l} 1 + \sum_{n=2} \frac{(n+1)(n+2)}{2n+1} a_n^2 - \\ -\frac{1}{3} \sum_{\substack{m,n,l=2 \\ i+j+k=2}}^{m,n,l=\infty} \begin{pmatrix} 3 \\ i\ j\ k \end{pmatrix} \langle m,n,l \rangle a_m^i a_n^j a_l^k \end{array} \right)$$

where:

$$\langle m,n,l \rangle = \int_0^\pi P_m(\cos\theta) P_n(\cos\theta) P_l(\cos\theta) \sin\theta \, d\theta$$

Considering only the mode $n=2$, at the second order accuracy, the dependence of the parameter β on time assumes the following expression:

$$\beta = \frac{A_{spheroid}}{A_{sphere}} = 1 + \frac{2}{5} a_{n,0}^2 \sin^2(\omega_2 t) \tag{6}$$

Quasi steady-state assumption

To apply the above found analytical solution for the evaporation rate (4), valid for steady conditions, to an oscillating drop, a quasi steady-state assumption is necessary. Such assumption may hold when the characteristic time scale of the oscillation process is much larger than that of the evaporation one. While the first one is easy to be defined as the inverse of the oscillation frequency:

$$t_{oscill} \approx \sqrt{\frac{\rho_l R_0^3}{\sigma}}$$

the evaporation time scale is not easily defined.

Evaporation is an overlapping of a diffusive phenomenon (driven by the coefficient D_v) and a convective one (i.e. the Stefan flow, driven by a characteristic velocity $U_0 = \frac{m_{ev}}{\beta 4\pi R_o^2 \rho} = \frac{\hat{m}_{ev}}{\beta} \frac{D_v}{R_0}$). From these two parameters and the drop size, three characteristic, but not independent, times (convective, diffusive and convective-diffusive) can be defined:

$$t_{conv} \approx \frac{R_0}{U_0}$$

$$t_{diff} \approx \frac{R_o^2}{D_v}$$

$$t_{cd} \approx \frac{D_v}{U_0^2} = \frac{t_{conv}^2}{t_{diff}}$$

Rearranging the previous definitions, the following correlation can be obtained:

$$t_{conv} \approx \frac{\beta R_0^2}{\hat{m}_{ev} D_v} = \frac{\beta t_{diff}}{\hat{m}_{ev}}$$

$$t_{cd} \approx \frac{\beta^2 R_0^2}{\hat{m}_{ev}^2 D_v} = \frac{\beta^2 t_{diff}}{\hat{m}_{ev}^2}$$

The quasi steady state assumption may be acceptable when:

$$t_{evap} \ll t_{oscill}$$

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where t_{evap} may be one of the three above mentioned characteristic times. An inspection on the values of such characteristic times shows that the inequality may acceptably hold for small drops (few tenths of micron) in hot gaseous environment and for hydrocarbon drops. But it may be questionable for larger drops, for lower gas temperature and for water drops.

Under this assumption, the above developed model can be applied to an oscillating drop. The total evaporated mass from a single oscillating drop during an oscillating period (assuming the time spent in prolate state equal to that spent in oblate state) can be calculated as:

$$M = \int_0^T m_{ev}\, dt = m_{ev,sphere} \int_0^T C\left(\beta(t)\right) dt =$$
$$= m_{ev,sphere} \left[\int_0^{T/2} C_{oblate}\left(\beta(t)\right) dt + \int_0^{T/2} C_{prolate}\left(\beta(t)\right) dt \right] \quad (7)$$

where $\beta(t)$ is given by equation (6).

PRELIMINARY RESULTS

Considering a single oscillating drop, the temporal evolution of instantaneous non-dimensional evaporation rate ($m_{ev}/m_{ev,sphere}$) can be related to the deformation status, as reported in Figure 3. The non-dimensional evaporation rate is always greater than 1, confirming that for an oscillating liquid drop the evaporation rate is always higher than that of the corresponding non-oscillating isovolumic spherical drop. Furthermore, when the drop is in the prolate state, its evaporation rate reaches the highest values.
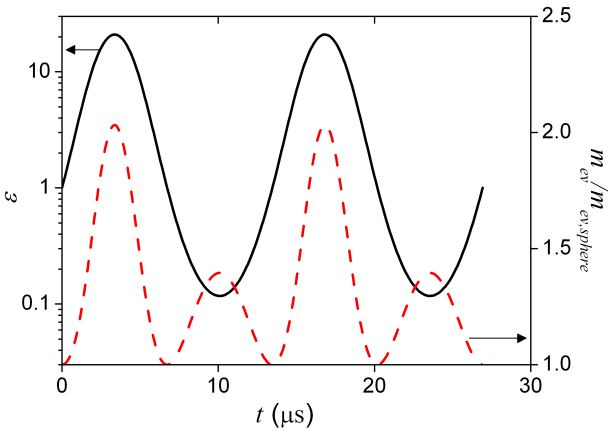

Figure 3: Temporal evolution of spheroid eccentricity (ε) and non-dimensional instantaneous evaporation rate ($m_{ev}/m_{ev,sphere}$) for a $R_0 = 10$ µm iso-octane drop.

The comparison between the evaporated mass from an oscillating drop and that from a spherical iso-volumic drop can be performed, for different values of the "excess" energy (defined as the kinetic energy associated to the oscillation modes), that can be easily related to the maximum drop surface area. The percentage difference in the evaporated mass, defined as:

$$\Delta ev\% = \frac{M - m_{ev,sphere} T}{m_{ev,sphere} T} 100$$

where M is calculated from equation (7) can be related to the percentage excess area $\left(\Delta\beta_{max}\% = (\beta_{max} - 1) 100\right)$ and Figure 4 reports the results for a 10 µm iso-octane drop in a

hot (700°C) gaseous environment. These preliminary results show that a simple correction for evaporation from oscillating drops could be implemented by assuming an approximate linear relation between the two parameters, where the proportionality coefficient may depend on drop and environment characteristics.
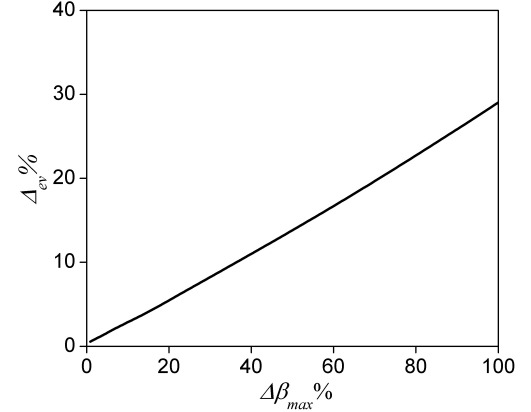

Figure 4: Percentage relative difference of evaporated mass as function of the maximum drop surface area ratio (in percentage).

CONCLUSIONS

Vapour and gas transport equations are analytically solved in oblate and prolate spheroidal coordinate systems, yielding the vapour distribution around a spheroidal drop and the surface flux under steady state conditions.

The drop evaporation rate can be defined as function of drop spheroidal shape and drop surface. Compared with iso-volumic spherical drop, spheroidal drops yield larger evaporation rate, with the oblate shape yielding a lower evaporation rate then the prolate one with the same surface area.

Application to oscillating drop is possible under quasi steady-state assumption, that may hold for small hydrocarbon drops in hot gaseous environment, yielding rather easy-to-implement corrections to the standard spherical case.

ACKNOWLEDGMENTS

NOMENCLATURE

Greek symbols

α	Species index	-
β	Surface ratio	-
Δ	Relative difference	-
ε	Spheroid eccentricity	-
ρ	Density	kg/m^3
ξ	Mass fraction	-
γ	Specie flux	kg/m^{2}s
σ	Surface tension	kg/s^2
ζ, ϕ, φ	Spheroid coordinates	-

ω	Oscillation frequency	1/s
Roman symbols		
a	Perturbation parameter	-
a_r, a_z	Radial and axial spheroid axes	m
C	Evaporation rate factor	
D_v	Diffusivity	m^2/s
M	Mass	kg
m_{ev}	Evaporation rate	kg/s
n	Oscillation mode	-
P_n	Legendre polynomials	-
R	Drop radius	m
t	Time	s
T	Oscillating period	s
U	Velocity	m/s
x, y, z	Cartesian coordinates	-
Subscripts		
$conv$	Convective	-
$diff$	Diffusive	-
cd	convective-diffusive	-
$evap$	Evaporation	-
g	Gaseous	-
l	Liquid	-
$oscil$	Oscillation	-
$0, s$	Surface	-
v	Vapour	-
∞	Infinity	-
Superscripts		
$\wedge$	Non-dimensional	-

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