



DROPLET EVAPORATION: CHARACTERISING FULLY TRANSIENT BEHAVIOUR IN THE GAS AND LIQUID PHASES

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ABSTRACT

We investigate the problem of a single, spherical, mono-component droplet evaporating in an infinite, quiescent, gaseous atmosphere by means of a comprehensive fully transient model. We present new findings concerning how the overall evaporation process is affected by retaining the often-neglected transient terms in the governing equations. The problem is solved numerically using a model that is validated by recovering known analytical solutions, and matching available experimental data.

Both transient terms in the gas and liquid phases can have a significant effect on the evaporation characteristics. Liquid phase transients refer to the droplet heating, or cooling, to the steady temperature, and gas phase transients refer to the cooling and saturating of the surrounding gas as the droplet releases vapour and absorbs heat from the environment. We find that transient terms in the gas phase can be responsible for up to a 43% reduction in evaporation time in extreme cases. A simple method to calculate this difference is presented. Incorporating transients in both the gas and liquid phases results in a significantly more complex problem. We demonstrate that there is a clear coupling between gas and liquid phases that eliminates the possibility to consider each phase in isolation. Importantly, it was found that differences in evaporation time caused by gas phase transients are even greater in the presence of droplet heating, compared to cases where droplet heating is negligible.

1. INTRODUCTION

The single evaporating droplet is a foundational problem of significant theoretical and practical importance. Models of more complex scenarios such as droplets in convective flows [1], or spray evaporation [2] are often extensions of solutions for the single droplet problem. Hence, advancing our understanding of this problem is important for a range of practical applications such as combustion, spray cooling, climate science, medicine delivery, and the current critically important application of virus transmission mechanisms.

Droplet evaporation is inherently a transient process. When a droplet is suddenly exposed to a gas (e.g. by injection), the droplet will heat, or cool, until the steady *wet-bulb* temperature $T_{s, QS}$ is reached. Simultaneously, vapour is liberated from the droplet surface and accumulates in the surrounding gas, and the region around the droplet is cooled, and heat is transported within the droplet. Another key transient process is the receding velocity of the droplet surface. These transient processes are often neglected to obtain the full quasi-steady (QS) solution, which results in the *d²-law* [3], meaning that the diameter-squared reduces linearly in time. This *d²-law* behaviour has been observed in many experiments [4]. Previous studies have investigated liquid phase transients (i.e. droplet heating), but while assuming that the gas is quasi-steady [5,6]. There are few studies that have included the gas phase transient terms, and those that do exist consider just a limited number of cases [7]. Here, we comprehensively investigate both the liquid and gas phase transients simultaneously. We model many cases in a dimensionless framework, which enables generalised conclusions to be drawn about how the transient terms influence evaporation.

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In this paper, we first define the problem and outline the governing equations, assumptions, and solution method. This is followed by key results when considering gas phase transients in isolation and then when gas and liquid phase transients are combined. Finally, conclusions are given.

2. MODEL DESCRIPTION

The problem being addressed is depicted in Figure 1. A single, spherical, mono-component droplet is evaporating in an infinite, quiescent, gaseous atmosphere. For given fluids and ambient far field conditions (temperature T_∞ , vapour concentration ω_∞ , and pressure P_∞), the task is to predict how the droplet radius a evolves over time. The problem governing equations and boundary conditions are now given while specifying all key assumptions. It is assumed that the gas is incompressible, and that gravitational forces, the Knudsen layer, viscous effects, and radiative heat transfer are negligible. These assumptions are generally valid for droplet sizes of 10^{-6} - 10^{-4} m [8]. By neglecting gravity, the problem becomes spherically symmetric, and incompressibility decouples the momentum equation. Therefore, the gas phase ($r > a$) is governed by the one-dimensional (radial), transient mass, species and energy equations, respectively given by

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho u) = 0 \quad (1)$$

$$\rho \left(\frac{\partial \omega}{\partial t} + u \frac{\partial \omega}{\partial r} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \Gamma \frac{\partial \omega}{\partial r} \right) \quad (2)$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial r} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \lambda \frac{\partial T}{\partial r} \right) + \Delta c_p \Gamma \frac{\partial \omega}{\partial r} \frac{\partial T}{\partial r} \quad (3)$$

where r is the radial distance from the droplet centre, t is time, ρ is density, u is velocity, ω is the mass fraction of the evaporating species A (so $1 - \omega$ is the mass fraction of the ambient species B), T is temperature, Γ is the mass diffusivity, λ is thermal conductivity, c_p is the local specific heat capacity, and Δc_p is the specific heat difference between the evaporating species A and ambient species B ($\Delta c_p = c_{p,A} - c_{p,B}$). The system is closed by the ideal gas equation of state, given by $P_\infty = \rho RT$, where P_∞ is the system pressure and is constant due to the incompressibility assumption, and R is the local specific gas constant and depends on the local concentration of vapour, $R = R_B + \omega(R_A - R_B)$.

It is assumed that convection is negligible within the droplet and thermal expansion is neglected such that the liquid density ρ_l is constant. Therefore, the liquid phase ($r \leq a$) requires only the transient energy equation, given by

$$\rho_l c_l \frac{\partial T}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \lambda_l \frac{\partial T}{\partial r} \right) \quad (4)$$

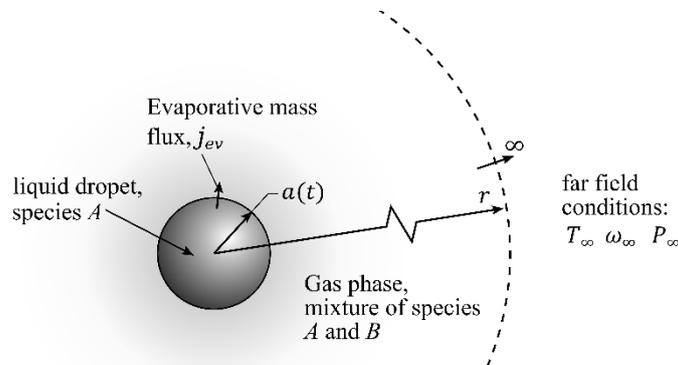


Figure 1: Problem illustration. A spherical, pure liquid droplet immersed in a gaseous environment extending to infinity.

where subscript l denotes liquid phase properties. All thermophysical properties are also assumed constant ($c_p, c_l, \lambda, \lambda_l, \Gamma$), which is valid if properties are evaluated at suitable average conditions [9].

The boundary conditions are as follows. The far field temperature and vapour concentration are fixed, i.e. $T \rightarrow T_\infty, \omega \rightarrow \omega_\infty$, for $r \rightarrow \infty$. Also, due to spherical symmetry, the temperature gradient at the droplet centre is zero, i.e. $\partial T / \partial r_{r=0} = 0$. Also, the ambient species B is insoluble in the droplet. This leads to an expression for the evaporative mass flux j_{ev} (the mass flux of species A across the surface) as

$$j_{ev} = -\frac{\Gamma}{1 - \omega_s} \left[\frac{\partial \omega}{\partial r} \right]_s \quad (5)$$

where subscript s denotes surface conditions ($r = a$). A mass balance across the surface yields the velocity of the droplet surface $\dot{a} = da/dt$ as

$$\dot{a} = -j_{ev} / \rho_l \quad (6)$$

Since the Knudsen layer is neglected, the temperature is continuous across the droplet interface such that $T_s^+ = T_s^-$ where superscript $+$ and $-$ indicate approaching the surface from the gas and liquid side respectively. Energy flux continuity across the surface yields

$$-\lambda_l \left[\frac{\partial T}{\partial r} \right]_s^- = -\lambda \left[\frac{\partial T}{\partial r} \right]_s^+ + j_{ev} \mathcal{L} \quad (7)$$

where \mathcal{L} is the latent heat of vaporisation. Finally, assuming local thermodynamic equilibrium at the droplet surface, the local vapour partial pressure $P_{s,A}$ is a function of the surface temperature T_s . This relationship is taken as the Clausius-Clapeyron equation

$$\frac{P_{s,A}}{P_\infty} = \exp \left[\frac{\mathcal{L}}{R_A} \left(\frac{1}{T_{sat}(P_\infty)} - \frac{1}{T_s} \right) \right] \quad (8)$$

where $T_{sat}(P_\infty)$ is the saturation temperature at P_∞ (i.e. the boiling point T_{BP}). The partial pressure $P_{s,A}$ may be converted to give the mass fraction of vapour at the surface ω_s .

Through dimensional analysis, the problem is shown to be fully described by eleven dimensionless groups: $Le = \lambda / (c_{p,\infty} \Gamma)$; $Ja = c_{p,A} T_{BP} / \mathcal{L}$; $\varepsilon = R_B / R_A$; $\bar{c}_p = c_{p,A} / c_{p,\infty}$; $\gamma = c_{p,A} / c_{v,A}$; $\bar{\rho} = \rho_\infty / \rho_l$; $\bar{c} = c_{p,\infty} / c_l$; $\bar{\lambda} = \lambda / \lambda_l$; $\mathcal{T} = T_\infty / T_{BP}$; $\Phi = 1 - \omega_\infty$. The final key parameter is the initial droplet temperature $\theta_o = (T_o - T_\infty) / (T_\infty - T_{s,QS})$, where T_o is the initial droplet temperature, T_∞ is the far-field temperature, and $T_{s,QS}$ is the quasi-steady surface temperature (wet-bulb). Therefore, $\theta_o = -1$ means that the droplet begins at the quasi-steady temperature, so droplet heating or cooling is not applicable. Further details are given in [8]. In terms of initial conditions, we select that the droplet begins with initial radius a_o and at uniform temperature θ_o , and the gas is initially uniform at the far-field temperature and vapour concentration. Note that initial fields are not applicable if the quasi-steady assumption is applied.

The problem is solved numerically for a domain spanning 10^3 times the droplet's initial size. A key feature of the solver is implementing a moving mesh to account for the shrinkage of the droplet (the moving boundary). It was verified that all solutions are independent of the spatial and temporal discretisation resolution [4]. The model was validated by recovering known analytical solutions (the d^2 -law, and the heated sphere problem), and by reproducing other fully transient results [7], and by closely matching known microgravity experiments [10].

3. RESULTS

3.1 Gas phase transients only

When the initial droplet temperature is $\theta_o = -1$, only gas phase transients are responsible for deviations from the d^2 -law because the liquid starts at the steady temperature. Figure 1a shows how the temperature field takes time to develop around the droplet. When the droplet is suddenly exposed to the hot atmosphere, a temperature layer grows around the droplet, while the droplet shrinks simultaneously. Since there is only a finite amount of energy they droplet can absorb before being completely vaporised, the droplet can only cool a finite region of gas. The initially large temperature gradient lead to fast evaporation compared to the quasi-steady solution (Figure 1b). However, the temperature layer established in the early stages remains into the late stages of evaporation and effectively insulates the droplet leading to slower evaporation rates. We see that a low temperature region remains even after the droplet has completely vaporised. In contrast, the quasi-steady case predicts that the thermal layer shrinks in proportion with the droplet size.

We define the parameter ϵ as the overall percentage difference in evaporation time between the quasi-steady solution and the solution with a transient gas phase. It was found that when $\theta_o = -1$, over an extremely wide range of conditions, ϵ can be closely predicted ($\pm 20\%$) using the readily calculable parameter defined as δ (Figure 1c) from

$$\epsilon = 0.779 \left(\frac{1}{1 - 0.706 \delta} - 1 \right) \quad (9)$$

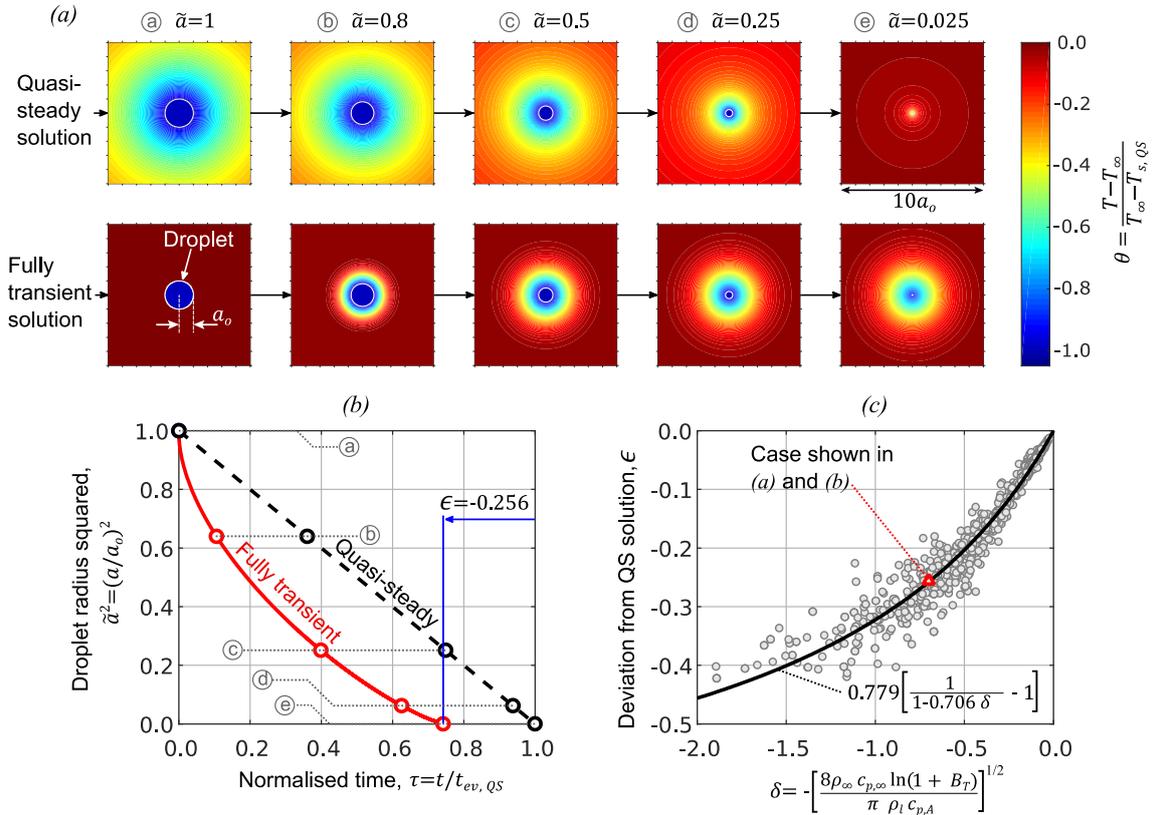


Figure 2: (a & b) Illustrative example results (inputs: $Le = 1$; $Ja = 2.5$; $\epsilon = 1$; $\bar{c}_p = 1$; $\gamma = 1.4$; $\bar{\rho} = 0.08$; $\bar{c} = 0.5$; $\bar{\lambda} = 0.2$; $T = 5$; $\Phi = 1$. This results in $B_T = 10.2$.) comparing fully transient model to quasi-steady model for sudden immersion where the droplet is initially at the wet-bulb temperature ($\theta_o = -1$). (a) Shows snapshots of cross-sections of the temperature field at various times, and (b) shows the droplet radius ‘a’ history. (c) Shows results for the deviation parameter ϵ against the dimensionless group δ for ~ 1000 cases. The specific case from (a & b) is shown by the red triangle on (c).

where

$$\delta = - \left[\frac{8\rho_\infty c_{p,\infty} \ln(1 + B_T)}{\pi \rho_l c_{p,A}} \right]^{1/2} \quad (10)$$

and $B_T = c_{p,A}(T_\infty - T_{s,QS})/\mathcal{L}$ is the Spalding heat transfer number. This significant result means that one can readily predict the difference between the steady and transient solutions without performing the computationally demanding fully transient solution.

3.2 Combined gas and liquid phase transients

While Figure 2 considers gas phase transients only (no droplet heating or cooling), Figure 3 shows the combined effects of gas and liquid phase transients. Of course, when the quasi-steady assumption is applied and the initial liquid temperature is $\theta_o = -1$, the d^2 -law is recovered. Including liquid phase transients only (known as the finite conductivity model), demonstrates slower evaporation as the droplet heats up and therefore a longer total evaporation time. Considering gas phase transients only obtains the characteristics shown previously in Figure 2 and the deviation ϵ_1 may be accurately predicted by equations (9) and (10).

However, when both gas and liquid phase transients are considered, a more complex coupling of the gas and liquid phases occurs. We find that the droplet surface initially heats up rapidly (Figure 3b) due to the very large temperature gradients from the ‘sudden immersion’ initial conditions. Then, as the surrounding gas cools and the heat progressively diffuses to the droplet centre, the droplet surface heats up much slower. The resulting effect on the droplet size history (Figure 3a) is that initially the evaporation rate is similar to the d^2 -law despite the much lower droplet temperature. However, as the gas field settles, the effect of the lower droplet temperature takes over and the evaporation rate is slower than the d^2 -law, and is more comparable to the liquid transients only case. In the final stages of evaporation, we again observe a reduction in evaporation rate as an insulating layer of cold vapour that was established in the early stages of evaporation surrounds the droplet (see Figure 2a).

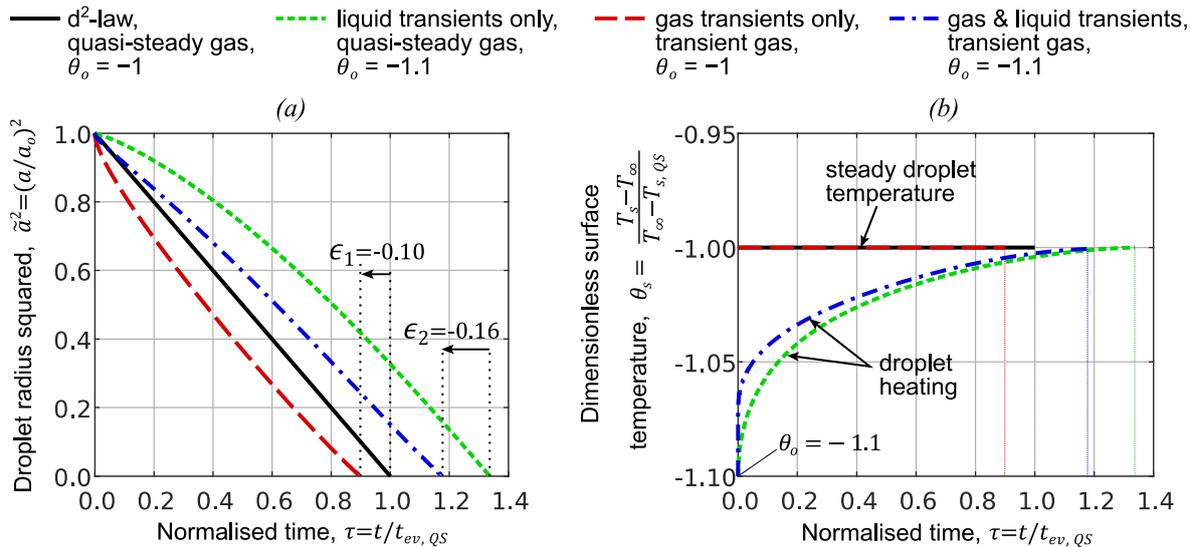


Figure 3: (a) Droplet radius history, and (b) dimensionless surface temperature history for a range of models. All models have the same governing parameters ($Le = 1$; $Ja = 2$; $\varepsilon = 1$; $\bar{c}_p = 1$; $\gamma = 1.4$; $\bar{\rho} = 0.01$; $\bar{c} = 0.4$; $\bar{\lambda} = 0.3$; $\mathcal{F} = 4$; $\Phi = 1$). The ‘quasi-steady’ and ‘gas transients only’ models start at the steady surface temperature ($T_s = T_{s,QS}$, $\theta_o = -1$) so do not include droplet heating, whereas the other two cases start at a lower temperature ($\theta_o = -1.1$) and must heat up to the steady temperature while evaporating.

On Figure 2a, the parameter ϵ_2 quantifies the deviation due to gas phase transients when liquid phase transients are also present. It is significant that $|\epsilon_2| > |\epsilon_1|$ since this means that the difference in evaporation time caused by including gas phase transients is significantly increased when liquid phase transients are also included. To our knowledge, this coupling effect between gas and liquid phase transients has not been previously reported. Although just one example case is shown here, this finding is robust across many cases. Therefore, this suggests that ϵ quantified by equation (9), which is valid for $\theta_o = -1$, underestimates the magnitude of ϵ when $\theta_o < -1$. When $\theta_o \neq -1$, the quantity ϵ also becomes a function of θ_o and the thermal conductivity and heat capacity ratios, $\bar{\lambda}$ and \bar{c} respectively.

4. CONCLUSIONS

A model for the single droplet evaporation problem has been developed that includes the often-neglected transient terms and, importantly, accounts for the receding surface velocity. The model is capable of recovering known theoretical results in limiting cases and is consistent with previous studies and experiments. The model has been used to investigate fully transient droplet evaporation characteristics, which have been shown to depend on eleven governing dimensionless groups when subject to the present assumptions. We revealed that, under certain conditions, gas phase transients can significantly affect the evaporation process. A simple method has been outlined to calculate the difference in evaporation time due to gas phase transients (quantified by ϵ), with good accuracy. The magnitude of ϵ is important for determining if one can apply the quasi-steady assumption, which significantly simplifies the problem. For small ϵ , the QS assumption is valid. If ϵ is large in magnitude, then either the fully transient solution is required, or the value of ϵ from equation (9) for example can be interpreted as a correction to evaporation time from the QS solution. Finally, it was shown that there exists a close coupling effect between the gas and liquid phases. Importantly, we showed that $|\epsilon|$ is greater when droplet heating is present, compared to gas phase transients in isolation. This fact should be considered when deciding if the quasi-steady assumption is valid.

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