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UNSTEADY DROPLET PHASE CHANGE IN THE PRESENCE OF CONVECTION

by

John K. Dukowicz

ABSTRACT

Simple expressions for the rate of change of droplet mass and droplet temperature are derived for an arbitrary convective environment, under the assumptions: (1) unity Lewis number, or constant Lewis number and equal gas-phase species C_p , and (2) uniform conditions on the droplet surface. Supplemented by a suitable droplet heat-flux correlation, these equations form a simple, but quite general, droplet phase change model.

1. INTRODUCTION

Single droplet evaporation or condensation is a fundamental phenomenon of interest in a wide variety of applications. In this paper we will develop a simple description of this phenomenon for use in a large numerical simulation code. Current models are based on analytical solutions of the spherically symmetric case in a quiescent environment (no convection) which is then modified by the use of a convection factor (sometimes called the ventilation or wind factor).^{1,2} However, the spherically symmetric case has some undesirable implications. For an evaporating droplet for which the ambient gas does not dissolve in the liquid, this solution constrains the flow in such a way that only the vapor is in motion. Hence, enthalpy transport is due only to the vapor and the solution depends on the vapor specific heat (C_p) and not the gas specific heat.³ In practice, spherical symmetry will be invariably destroyed either by a nonspherical droplet shape, or by the presence of even minute amounts of free convection. This constraint, therefore, is generally absent and the consequences which are embodied in the solution can be misleading. Thus, although

the spherically symmetric solution provides much physical insight, the results will not be generally useful without modification.

For a more general solution the associated flow field must be obtained, which is generally not feasible. However, the details of such a solution are frequently not required. What is needed for a complete model of droplet evaporation or condensation, and its interaction with the environment, is the total rate of change of droplet mass and the rate of change of droplet temperature. This can be obtained under quite general conditions, in terms of the heat flux to the droplet, by exploiting the well-known analogy between heat and mass transfer.

The common formulation of this analogy⁴ is restricted to low mass transfer rates. The analogy is therefore reformulated in more general terms to show that an exact analogy is possible when conditions on the droplet surface are uniform and Lewis number is unity. Further, a partial analogy is shown to exist when Lewis number differs from unity but when all the species enthalpies are equal. In both cases the properties of the analogy are used to relate the vapor mass flux at the droplet surface to the temperature gradient, and therefore obtain the droplet evaporation rate in terms of the conduction heat flux to the droplet. Since satisfactory experimental heat flux correlations are available for droplets, these relationships constitute a complete model for droplet phase change.

The results are found to vindicate the use of the ventilation factor to modify the non-convective solution, except that in the present case the ventilation factor appears naturally as part of the heat flux correlation. Further, the results are consistent with the spherical solution, provided gas enthalpies are appropriately interpreted.

II. DROPLET EVAPORATION

A. General

The droplet energy equation in its fundamental form can be written as follows

$$\frac{d}{dt} (m \langle h_d \rangle) = h_{vs} \frac{dm}{dt} + Q \quad , \quad (1)$$

where m is the droplet mass, $\langle h_d \rangle$ is the average droplet specific enthalpy (assuming temperature inside the droplet is not uniform), h_{vs} is the vapor enthalpy at the surface and Q is the total heat flux supplied by the gas to the droplet. Alternatively this equation can be written as

$$\frac{d}{dt} (m \langle h_d \rangle) - h_{ds} \frac{dm}{dt} = L \frac{dm}{dt} + Q \quad , \quad (2)$$

where $L = h_{vs} - h_{ds}$ is the latent heat. In the simple case when the droplet temperature is uniform, the energy equation takes the familiar form

$$m C_d \frac{dT_d}{dt} = L \frac{dm}{dt} + Q \quad , \quad (3)$$

where C_d is the droplet specific heat and T_d is the droplet temperature. In thermal equilibrium the droplet temperature does not change, and all the heat supplied to the droplet goes into supplying the latent heat ($L \, dm/dt = -Q$). However, when the droplet is not in thermal equilibrium only part of the heat supplied (Q) goes into latent heat, and the rest is used to change the droplet temperature, as expressed by Eq. (3).

The more general equation can be written in the form

$$m \langle C_d \rangle \frac{dT_d}{dt} = L \frac{dm}{dt} + Q \quad , \quad (4)$$

where

$$\langle C_d \rangle = \frac{d\langle h_d \rangle}{dT_s} + \frac{(\langle h_d \rangle - h_{ds})}{m} \frac{dm}{dT_s} \quad (5)$$

is an average specific heat for the droplet. In the following discussion it will be convenient to use Eq. (4), restricting it to the case of uniform droplet temperature, since in practice the more general form can always be used, together with some model for the internal droplet temperature distribution.

We now assume that the conditions on the droplet surface are uniform. This assumption will be essential later to demonstrate the analogy. Under conditions of strong convection, surface temperatures would be expected to vary unless there is strong internal circulation (good mixing) or where the droplet is so small that internal thermal diffusivity will maintain uniform surface temperature. We consider the droplet to be evaporating into a non-condensable gas. We therefore deal with a two-component system in the gas-phase, composed of the vapor and the non-condensable gas, even though each component may consist of a mixture of different species.

It is convenient to introduce the local surface heat flux (q_s) and the vapor mass flux (F_{vs}) such that, because of the uniformity of droplet surface conditions, we can write

$$\dot{Q} = - A q_s$$

and

$$\frac{dm}{dt} = - A F_{vs}$$

where A is the droplet surface area. In terms of these fluxes, the governing equations are

$$\frac{dm}{dt} = Q \frac{F_{vs}}{q_s} \tag{6}$$

and

$$m\langle C_d \rangle \frac{dT_s}{dt} = Q \left(1 + L \frac{F_{vs}}{q_s} \right) . \quad (7)$$

These are the equations that define the droplet transient, provided Q and F_{vs}/q_s are known. In the following, we will show how these quantities are to be determined.

The ratio of fluxes at the droplet surface F_{vs}/q_s can be re-expressed as follows. The component mass flux at the droplet surface is

$$F_{is} = (\rho_i u_i - \rho D \nabla Y_i)_s ,$$

neglecting the droplet surface regression rate (hence assuming subcritical temperatures and pressures), and where D is the binary diffusion coefficient between the vapor and the gas. If we assume that the gas is insoluble in the droplet, then the mass flux of the gas relative to the droplet surface is zero ($F_{gs} = 0$) and therefore

$$F_{vs} = - (\rho D)_s \frac{\nabla Y_{vs}}{1 - Y_{vs}} . \quad (8)$$

Since the heat flux at the surface is

$$q_s = - k_{s-s} \nabla T_s , \quad (9)$$

the ratio of fluxes becomes

$$\frac{F_{vs}}{q_s} = \left(\frac{\rho D}{k} \right)_s \frac{1}{1 - Y_{vs}} \frac{\nabla Y_{vs}}{\nabla T_s} , \quad (10)$$

which is a scalar expression because the gradients are colinear at the droplet surface. This expression has to be quantitatively evaluated by means of the analogy which is developed below.

B. Development of the Heat-Mass Transfer Analogy

The analogy between heat and mass transfer is based on the similarity of the differential equations and boundary conditions specifying the two problems. Most frequently the analogy is developed for a simplified set of equations, namely equations valid for a predominant single component and for constant property conditions, and the results are used to deduce relationships between the respective transfer coefficients.^{4,5} In the present case we wish to generalize the analogy to apply to a multi-component system, so that strong mass transfer is not excluded. We also do not wish to exclude variable properties.

The analogy can be shown to exist only for the steady-state gas phase equations. However, except near critical droplet temperatures and pressures, gas phase transfer rates are so much faster than liquid-phase transfer rates that essentially quasi-steady conditions can be assumed to exist to the gas-phase. This is the basis for the many quasi-steady theories of evaporation in the literature.² The accuracy of the quasi-steady assumption has been numerically verified under plausible conditions⁶.

The relevant differential equations are the species continuity equation and the energy equation. In the absence of chemical reactions, the species continuity equation can be written in the form⁴

$$\rho \mathbf{u} \cdot \nabla \mathbf{Y}_i = \nabla \cdot \rho D \nabla \mathbf{Y}_i \quad , \quad (11)$$

where, as is usual, this equation neglects pressure, thermal and forced diffusion.

The energy equation can be written in general⁴ as

$$\rho \mathbf{u} \cdot \nabla h = - \nabla \cdot \mathbf{q} + \mathbf{u} \cdot \nabla p - \tau : \nabla \mathbf{u} \quad , \quad (12)$$

where h is the total specific enthalpy

$$h = \sum_i Y_i h_i, \quad (13)$$

and $\tilde{q}$ is the total heat flux given by

$$\tilde{q} = - \tilde{k} \tilde{\nabla} T - \rho D \sum_i h_i \tilde{\nabla} Y_i, \quad (14)$$

where, as usual, the thermo-diffusion (Dufour) effect is neglected. The last term in this equation is the enthalpy diffusion term. This term is significant at the droplet surface since frequently the gas component is not soluble in the droplet and its velocity relative to the droplet surface is zero. This means that there is inherently a large difference between the vapor and gas velocities at the droplet surface, and hence a large effect of thermal diffusion. For the case of droplet evaporation, where local velocities are relatively low, pressure may be considered constant^{2,6} and viscous dissipation is not important. In such a case, the last two terms of Eq. (12) are neglected and the energy equation becomes

$$\rho \tilde{u} \cdot \tilde{\nabla} h = \tilde{\nabla} \cdot \tilde{k} \tilde{\nabla} T + \tilde{\nabla} \cdot \rho D \sum_i h_i \tilde{\nabla} Y_i. \quad (15)$$

We can eliminate the temperature by differentiating Eq. (13) to get

$$\tilde{\nabla} h = C_{p\sim} \tilde{\nabla} T + \sum_i h_i \tilde{\nabla} Y_i \quad (16)$$

where $C_p + \sum_i Y_i C_{pi}$, and $C_{pi} = \left. \frac{\partial h_i}{\partial T} \right|_p$ is the specific heat at constant pressure of component i . The resulting energy equation is

$$\rho_{\tilde{u}} \cdot \tilde{\nabla} h = \tilde{\nabla} \cdot \frac{k}{C_p} \tilde{\nabla} h + \tilde{\nabla} \cdot \left(\rho D - \frac{k}{C_p} \right) \sum_i h_i \tilde{\nabla} Y_i \quad . \quad (17)$$

This equation simplifies under two conditions:

- (1) If $\rho D = \frac{k}{C_p}$, or equivalently $Le = \frac{\rho D C_p}{k} = 1$, the energy equation becomes

$$\rho_{\tilde{u}} \cdot \tilde{\nabla} h = \tilde{\nabla} \cdot \rho D \tilde{\nabla} h \quad . \quad (18)$$

- (2) If $h_i = h$, or equivalently $C_{pi} = C_p$, the energy equation becomes

$$\rho_{\tilde{u}} \cdot \tilde{\nabla} h = \tilde{\nabla} \cdot \frac{\rho D}{Le} \tilde{\nabla} h \quad . \quad (19)$$

Notice that Eq. (18) is exactly of the same form as Eq. (11), while Eq. (19) is similar but differs in the magnitude at the effective diffusivity whenever Le is different from unity.

To demonstrate the analogy we must assume that conditions on the droplet surface are uniform. Given a uniform surface temperature, we define scaled variables

$$Y_i^* \equiv \frac{Y_i - Y_{is}}{Y_{i\infty} - Y_{is}} \quad ,$$

and (20)

$$h^* \equiv \frac{h - h_s}{h_\infty - h_s} \quad .$$

In terms of these variables the equations become

$$\rho_{\tilde{u}} \cdot \nabla \tilde{Y}_i^* = \tilde{\nabla} \cdot \rho D \tilde{\nabla} \tilde{Y}_i^* \quad , \quad (21a)$$

$$\rho_{\tilde{u}} \cdot \nabla \tilde{h}^* = \tilde{\nabla} \cdot \rho D \tilde{\nabla} \tilde{h}^* \quad , \quad (21b)$$

$$\rho_{\tilde{u}} \cdot \nabla \tilde{h}^* = \tilde{\nabla} \cdot \frac{1}{Le} \rho D \tilde{\nabla} \tilde{h}^* \quad , \quad (21c)$$

and the boundary conditions are

$$\tilde{Y}_{is}^* = \tilde{h}_s^* = 0 \quad \text{for } \tilde{r} = \tilde{r}_s$$

$$\tilde{Y}_{i\infty}^* = \tilde{h}_{\infty}^* = 1 \quad \text{for } \tilde{r} \rightarrow \infty$$

For case (1) (i.e., $Le = 1$) the analogy is exact. That is, both the boundary conditions and the differential equations are the same, and therefore,

$$\tilde{Y}_i^* = \tilde{h}^* \quad ,$$

or

$$\frac{\tilde{Y}_i - \tilde{Y}_{is}}{\tilde{Y}_{i\infty} - \tilde{Y}_{is}} = \frac{\tilde{h} - \tilde{h}_s}{\tilde{h}_{\infty} - \tilde{h}_s} \quad .$$

Note that this result holds for the case of variable diffusivity, and an arbitrary geometry and flow field. Essentially the same result was derived for the steady boundary layer equations by Lees⁷ and Eckert and Drake.⁸

Next, for case (2) (i.e., $C_{pi} = C_p$) the analogy is only partial since the differential equations are similar but not identical. We can make progress, however, if we assume that the Lewis number, while different from unity, is a constant throughout the flow field. This is frequently a good assumption, especially for the single component case. With this assumption, Eq. (21c) becomes

$$\rho_{\sim} \mathbf{u}_{\sim} \cdot \nabla_{\sim} h^* = \eta \nabla_{\sim} \cdot \rho D \nabla_{\sim} h^* \quad , \quad (22)$$

where $\eta = 1/Le$. Introducing the transformation

$$\mathbf{r}' = \eta^{-1/2} \mathbf{r} \quad ,$$

$$u'(\mathbf{r}') = \eta^{-1/2} u(\mathbf{r}) \quad ,$$

the energy equation becomes

$$\rho_{\sim} \mathbf{u}' \cdot \nabla' h^* = \nabla' \cdot \rho D \nabla' h^* \quad , \quad (23)$$

where the gradient ∇' operates with respect to the transformed coordinate $\mathbf{r}'$. Comparing Eq. (23) with Eq. (21a), we see that a modified analogy applies, namely

$$h^*(\mathbf{r}; u(\mathbf{r})) = Y_i^*(\mathbf{r}'; u'(\mathbf{r}')) = Y_i^*(\eta^{-1/2} \mathbf{r}; \eta^{-1/2} u(\mathbf{r})) \quad , \quad (24)$$

where the notation used means that $h^*(\mathbf{r}; u(\mathbf{r}))$ is a function of $\mathbf{r}$ corresponding to the velocity field $u(\mathbf{r})$. Alternatively, we can write

$$Y_i^*(r; u(r)) = h^*(\eta_i^1 r; \eta_i^2 u(r)) \quad . \quad (25)$$

This result can be easily verified for the steady-state, constant property, spherically symmetrical solution².

C. Evaporation Model (Le = 1)

For this case we find

$$\tilde{r}_h = \left[\frac{h_\infty - h_s}{Y_{v\infty} - Y_{vs}} \right] \tilde{\nabla} Y_v \quad .$$

Using Eq. (16), the temperature gradient is

$$\tilde{\nabla} T = \left[\frac{h_\infty - h_s}{Y_{v\infty} - Y_{vs}} \right] \frac{\tilde{\nabla} Y_v}{C_p} - \sum_i \frac{h_i}{C_p} \tilde{\nabla} Y_i \quad .$$

At the droplet surface, for the case of two components, we have

$$\tilde{r}_s T = \left(\frac{h_\infty - h_s}{Y_{v\infty} - Y_{vs}} - h_{vs} + h_{gs} \right) \frac{\tilde{\nabla} Y_v}{C_{ps}} \quad .$$

Finally, from Eq. (10), the flux ratio is

$$\frac{F_{vs}}{q_s} = - \left(\frac{\rho D C_p}{k} \right)_s \frac{B_Y}{h_\infty - h_s - (h_{vs} - h_{gs})(Y_{v\infty} - Y_{vs})} \quad , \quad (26)$$

or alternatively

$$\frac{F_{vs}}{q_s} = - \left(\frac{\rho DC_p}{k} \right)_s \frac{B_Y}{h_{g^\infty} - h_{gs} + (h_{v^\infty} - h_{vs} - h_{g^\infty} + h_{gs}) Y_{v^\infty}} \quad (27)$$

where

$$B_Y = (Y_{vs} - Y_{v^\infty}) / (1 - Y_{vs}) \quad (28)$$

is the mass transfer number.²

These results are exact for the case $Le = 1$. For consistency, the factor $Le = \rho DC_p / k$, evaluated at the surface, should be set to unity. However, anticipating the results of the next section, this factor may be retained to partially account for the effects of a Lewis number different from unity.

Thermal equilibrium will occur when the droplet temperature no longer changes in time. Therefore, the wet-bulb temperature is determined by setting the right hand side of Eq. (7) to zero,

$$1 + L \frac{F_{vs}}{q_s} = 0 \quad .$$

In the interesting case when $Y_{v^\infty} = 0$, the wet-bulb temperature is given by

$$B_Y = \frac{Y_{vs}}{1 - Y_{vs}} = \left(\frac{k}{\rho DC_p} \right)_s \frac{h_{g^\infty} - h_{gs}}{L} \quad (29)$$

This is an implicit relationship for the wet-bulb temperature since the surface vapor mass fraction is given by the vapor-pressure relationship at surface temperature. This is a general result which illustrates one distinctive result of the present theory since, while it is similar to those seen in the literature,¹⁻³ it is the gas enthalpy difference that appears, in contrast to the spherically

symmetric solution which suggests that the vapor enthalpy difference should be used.³

D. Evaporation Model ($C_{pi} = C_p$)

Differentiating both sides of Eq. (24) at the droplet surface, we find

$$\frac{\partial Y_v}{\partial s} = - \frac{Th^*}{r_s^2} \frac{\partial r_s}{\partial s} \quad (25)$$

Using Eq. (16) and (20) this is rewritten

$$\frac{\partial Y_v}{\partial s} = C_{ps} \frac{Y_{v\infty} - Y_{vs}}{h_v - h_s} \frac{\partial T}{\partial s} \quad (26)$$

For this case, therefore, the mass fraction gradient is related to the temperature gradient for a scaled droplet size and velocity field.

Let us now assume that the heat transfer coefficient can be correlated using the generalized Frossling equation.⁹

$$Nu = 2 + K Re^m Pr^n \quad (30)$$

where K , m , n are experimentally determined. The use of such a steady-state correlation for an evaporating droplet can again be justified by arguments invoked previously for the existence of a quasi-steady state. For spherical droplets the correlation parameters are approximately $K = 0.6$, $m = 1/2$, and $n = 1/3$.⁵ This correlation implies that the surface temperature gradient is given by

$$\frac{\partial T}{\partial s} = \frac{k_r}{k_s} \frac{(T_\infty - T_s)}{2r_s} (2 + K Re^m Pr^n) \quad (31)$$

For the scaled droplet radius and velocity, we have

$$\frac{T_s - Y_{vs}}{T_\infty - T_s} = \frac{(Y_{vs} - Y_{\infty})}{2r_s} \frac{C_{ps} (T_\infty - T_s)}{(h_\infty - h_s)} \frac{k_r}{k_s} (2 + K Re^m Sc^m Pr^{n-m}) \quad (32)$$

Notice that the corresponding Sherwood number is

$$Sh = 2 + K Re^m Sc^m Pr^{n-m} \quad .$$

If this is to be analogous to Eq. (30), and therefore independent of Pr , we must have $n = m$. Since $m = 1/2$ is theoretically and experimentally well established,¹ this theory predicts

$$n = m = 1/2 \quad . \quad (33)$$

However, Frossling⁹ showed experimentally that $n = 1/3$. This can also be predicted theoretically under certain conditions, as discussed by Fuchs,¹ and has to do with a nonuniform distribution of temperature around the droplet surface, which violates the assumptions of the present theory. The difference is small in general. Since K is known to an accuracy of only about 10%,² this uncertainty is equivalent to a range of Prandtl and Schmidt numbers given by

$$0.75 < Pr, \quad Sc < 1.8 \quad .$$

Finally, taking the ratio of Eqs. (31) and (32), the flux ratio given by Eq. (10) becomes

$$\frac{F_{vs}}{q_s} = - \left(\frac{\rho DC_p}{k} \right)_s \left[\frac{2 + K Re_s^{-1} Sc_s^{-1}}{2 + K Re_s^{-1} Pr_s^{-1}} \right] \frac{B_Y}{h_\infty - h_s} \quad (34)$$

Comparing this with Eqs. (26) and (27), the direct effect of Lewis number appears in the leading factor, which occurs in both cases. Furthermore, for large Reynolds numbers, the factor arising from the correlations can deviate from unity and contributes an additional factor of $Le^{-1/2}$.

Finally, an obvious generalization that combines both special cases is

$$\frac{F_{vs}}{q_s} = - \left(\frac{\rho DC_p}{k} \right)_s \left[\frac{2 + K Re_s^{-1} Sc_s^{-1}}{2 + K Re_s^{-1} Pr_s^{-1}} \right] \frac{B_Y}{h_\infty - h_s - (h_{vs} - h_{gs})(Y_{\infty} - Y_{vs})} \quad (35)$$

Together with Eqs. (6) and (7), this constitutes a model for droplet evaporation, which can be integrated provided the heat flux Q is given. For spherical droplets, the heat flux can be obtained from heat-transfer coefficient correlations. The same argument employed previously, regarding the quasi-steady nature of the gas-phase, can be used to justify using the steady-state correlations. There are a number of correlations available for this purpose. For example, the well-established Ranz-Marshall⁵ correlation gives

$$Q = 2 \pi r_s k_r (T_\infty - T_s) (2 + 0.6 Re_s^{1/2} Pr_s^{1/3}) \quad (36)$$

where the reference temperature for evaluating transport properties is the average temperature, $(T_\infty + T_s)/2$. At free stream temperatures above 150°C, Yuen and Chen¹⁰ correlate their results with

$$Q = 2 \pi r_s k_s (T_\infty - T_s) (2 + 0.6 Re_s^{1/2} Pr_s^{1/3}) / B_E \quad (37)$$

where B_E is a correction for the effect of evaporation, given by

$$B_E = 1 + (h_v - h_g)/L \quad . \quad (38)$$

The transport properties are evaluated at surface temperature. Faeth,² on the other hand, proposes

$$B_E = B_Y / [n(1 + B_Y)] \quad (39)$$

so that the correlation gives the right limit for a motionless drop.

III. SUMMARY

Current models of single droplet evaporation are based on spherically symmetric, often constant property solutions, which are then modified by the use of a convection or ventilation factor. Since a spherically symmetric configuration constrains the flow in such a way that the solution depends on the enthalpy of the vapor only, and not on that of the gas,³ such a strictly geometrical result is unrealistic in other configurations and can lead to substantial error in the calculated evaporation of polyatomic substances, such as water, or many of the hydrocarbon fuels, whose vapor enthalpy is substantially greater than the enthalpy of air.

We have been able to largely relax the assumptions of a spherically symmetric flow field and the absence of convection, to produce an improved, but still simple evaporation model summarized by the following equations, given previously.

$$\frac{dm}{dt} = Q \frac{F}{q_s} \quad (6)$$

$$m < C_d > -\frac{dT_s}{dt} = Q \left(1 + L \frac{F}{q_s} \right) \quad (7)$$

$$\frac{F_{vs}}{q_s} = - \left(\frac{\rho DC_p}{k} \right)_s \left[\frac{2 + K Re_s^{-1} Sc_s^{-1}}{2 + K Re_s^{-1} Pr_s^{-1}} \right] \frac{B_Y}{h_\infty - h_s - (h_{vs} - h_{gs})(Y_{\infty} - Y_{vs})} \quad (34)$$

Given ambient and initial conditions, these equations can be numerically simultaneously integrated to provide droplet radius and temperature time histories.

The main assumptions employed to derive this model are

- (a) quasi-steady gas phase;
- (b) uniform surface conditions;
- (c) constant Lewis number;
- (d) spherical droplets, where available empirical correlations are used to evaluate Q .

Finally, it should be pointed out that these results vindicate the use of the ventilation factor to modify the non-convective (spherically-symmetric) solution, except that in this case the ventilation factor appears naturally as part of the heat flux correlation. Further this model is essentially consistent with the spherically symmetric model, provided the gas specific heats are appropriately interpreted.

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