Analytical Investigation of Lewis Number Effects on Non-Equilibrium Droplet Evaporation

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Abstract: Non-equilibrium phenomena have wide applications in real systems. Among these phenomena, non-equilibrium evaporation is a very common and important phenomenon especially in combustion. Although droplet size doesn't play a significant role in equilibrium approach, but has a considerable influence in non-equilibrium case. Non-equilibrium effects become significant when the initial droplet diameter is less than 100 μm, also for neglecting the effects of surface tension this diameter should be considered greater than 0.1 μm. Rate of droplet evaporation is also characterized by a Peclet Number which its difference from equilibrium Peclet Number is an indicator of the evaporation deviation from equilibrium. In this paper, the Lewis number effects on non-equilibrium evaporation of small droplet in a quiescent air are investigated theoretically. Therefore for different Lewis number, the Peclet Number and physical properties of the gas mixture surrounding the droplet including specific enthalpy, mass concentration, density and diffusion coefficient are reported.

Key words: Non-equilibrium · Droplet evaporation · Lewis number · Analytical model

INTRODUCTION

Non-equilibrium phenomena have wide applications in real systems. Living state is such a typical non-equilibrium state. These have relevance in physiology, geology, physical science and biological science, economics and social dynamics. There was tremendous interest in mid-twentieth century in exploring general principles for understanding non-equilibrium phenomena along with the development of non-equilibrium thermodynamics and non-equilibrium statistical mechanics. Pioneering work of Prigogine and his school in Brusels stimulated a good deal of interest in the field of non-equilibrium statistical mechanics [1].

Among these non-equilibrium phenomena, evaporation is very important, especially in combustion. For examples, in order for a fuel such as gasoline to burn, it must be evaporated. Liquid gasoline does not burn, only the vapors of fuel do. As we know, energy is the key research subject in the world and the base of all civilization. The most part of the world's energy is supplied by the combustion of fuels such as gasoline, heavy oils, coal and natural gas [2].

Droplet evaporation is also important in many devices, such as diesel engines, liquid–fuel rocket engines, aircraft jet engines and industrial furnaces. During spray combustion in such devices, fuel droplets are injected into the combustion chamber in liquid form and most of the droplets evaporate before combustion takes place. The concentration of the fuel vapor is determined by the evaporation rate of the droplets and it affects in performance of the combustion system significantly [3].

The problems of droplet heating, evaporation and ignition of fuel vapor/ air mixture have been widely discussed in literature [4-13].

Evaporation under terrestrial conditions is strongly influenced by gravity induced thermo-convective flows. Those effects mask the influence of non-equilibrium processes in phase transitions and make the proper understanding of the phenomenon very difficult in the ground-based experiments. Besides, non-equilibrium effects have a stronger manifestation for the droplets of small radius [14]. To determine droplet evaporation rate and combustion in microgravity experiments one needs for experimental data processing an adequate theoretical model accounting for non-equilibrium effects [15, 16].

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A great number of modeling studies for better understanding of vaporization and combustion of a fuel droplet under microgravity conditions have been reported for nearly five decades. Godsave [17] and Spalding [18] derived the classical d²-law, which yields relatively good estimates of the gasification rate. Kumagai *et al.* [19-21] successfully performed the first droplet combustion experiments in microgravity conditions to validate d²-law. They showed that droplet gasification rate was constant over time which is one of the most important features of d²-law.

In most models of droplet evaporation, it is assumed that the ambient gas is ideal. This assumption becomes questionable when the pressures are high enough, as observed in internal combustion engines. The main approaches to taking into account 'real gas' effects have been discussed in [22-26].

As we know, Soret and Dufour effects which is described as a flow of matter caused by a temperature gradient (thermal diffusion) and flow of heat caused by concentration gradients, respectively, occur simultaneously. Both effects are believed to be small in most cases, although sometimes their contribution may be significant [27-30].

In this work, non-equilibrium evaporation of small droplet is developed by considering effects of the Lewis number (i.e. a ratio of thermal diffusivity to mass diffusivity). This development is actually an extension of a similar work by Smirnov *et al.* [14]. Rate of droplet evaporation is characterized by a Peclet Number which its difference from equilibrium one is characterizing the deviation of evaporation from equilibrium. Here the physical properties variations of the gas mixture surrounding the droplet, such as specific enthalpy, mass concentration, density, diffusion coefficient and also Peclet Number with Lewis number are discussed and analyzed.

Mathematical Model for Non-Equilibrium Evaporation:
For modeling the non-equilibrium evaporation of a single droplet in a nonconvective atmosphere at a given temperature and pressure, this problem is considered as a quasi-steady state. Thus, the droplet is of fixed size and retains that size by a steady flux of fuel. One can consider the regression as being constant, or, even better, one can think of the droplet as a porous sphere being fed from a very thin tube at a rate equal to the mass evaporation rate so that the surface of the sphere is always wet and any liquid evaporated is immediately replaced. The porous sphere approach shows that a bulk
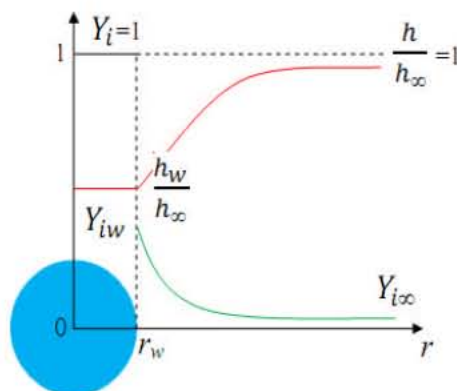

Fig. 1: The schematic radial profiles of specific enthalpy and mass fraction of the volatile component, in a droplet evaporation process

gaseous velocity outward must exist and this velocity in the spherical geometry will vary radially. With this physical consideration one may take the temperature throughout the droplet as constant and equal to the surface temperature as a consequence of the quasi-steady assumption [31]. Here the effects of Soret and Dufour are also neglected, the pressure is constant and there is no relative velocity between droplet and surrounding gas.

Two possible sources for internal motion within droplet evaporation are shear stress at the droplet surface and surface tension gradients [32]. In this model the droplet is small enough to neglect the former and evaporation takes place in non-convective atmosphere led to neglect the latter. The lack of internal motion in the droplet implies the spherical symmetry assumption.

Fig. 1 shows a schematic radial profiles for the mass fraction and specific enthalpy fields. By considering axi-symmetrical coordinates which its center is located in the center of the droplet, the problem is divided into two zones. First zone ($0 < r < r_w$), represents area occupied by liquid and the second zone ($r > r_w$), represents area occupied by gas mixture. Also $r = r_w$ denotes the interface between these two zones. By considering steady state and non-equilibrium evaporation of droplet which is heated uniformly, governing equations can be obtained.

The equations for the gas mixture above the interface ($r > r_w$) are:

$$\frac{d}{dr}\left(\rho v r^2\right) = 0 \qquad (1)$$

$$\rho v \frac{dY_i}{dr} = \frac{1}{r^2}\frac{d}{dr}\left(\rho r^2 D_i \frac{dY_i}{dr}\right), \quad i = 1,2,...,N \qquad (2)$$

$$\rho v \frac{dh}{dr} = \frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{\lambda}{c_p} \frac{dh}{dr}\right) \qquad (3)$$

$$P = \rho \frac{R}{m} T = \rho R T \sum_{i=1}^{N} \frac{Y_i}{m_i} = cont \qquad (4)$$

and for the liquid ($0 < r < r_w$)

$$Y_{nl} = 1, \qquad Y_{il} = 0, \qquad i = 1,2,...,N{-}1 \qquad (5)$$

$$T = T_w \qquad (6)$$

The boundary conditions at phase interface $r = r_w$ take the form

$$(\rho v)_g = (\rho v)_l = \dot{m} \qquad (7)$$
$$\dot{m} Y_{ig} = \left(\rho D_i \frac{dY_i}{dr}\right)_g \qquad (8)$$

$$\dot{m}(Y_{Ng} - 1) = \left(\rho D_N \frac{dY_N}{dr}\right)_g \qquad (9)$$

$$h_l \dot{m} = \left(\lambda \frac{dT}{dr}\right)_g \qquad (10)$$

and at infinity ($r \to \infty$)

$$T = T_e, \qquad Y_i = Y_{ie}, \qquad i = 1,2,...,N \qquad (11)$$

From Eq. (1) and the boundary condition (7) yield

$$?v = \dot{m}\frac{r_w^2}{r^2} \qquad (12)$$

For simplifying equations and boundary conditions, following dimensionless variables are introduced.

$$\bar{r} = \frac{r}{r_w}, \ \bar{h} = \frac{h}{h_e}, \ \bar{h}_l = \frac{h_l}{h_e}, \ Pe = \frac{\dot{m} r_w}{?D}, \ \bar{\rho} = \frac{\rho}{\rho_e}, \ \bar{D} = \frac{D}{D_e} \qquad (13)$$

Equations and boundary conditions are non-dimensionalized as

$$\frac{dY_i}{d\bar{r}} = \frac{d}{d\bar{r}} \frac{\bar{r}^2}{Pe} \frac{dY_i}{d\bar{r}}, \ i = 1,2,...,N \qquad (14)$$

$$\frac{d\bar{h}}{d\bar{r}} = \frac{d}{d\bar{r}} \frac{Le \bar{r}^2}{Pe} \frac{d\bar{h}}{d\bar{r}} \qquad (15)$$

$$\bar{r} = 1 : Y_{iw} = \left(\frac{1}{Pe}\frac{dY_{ig}}{d\bar{r}}\right)_w, \ Y_{Nw} - 1 = \left(\frac{1}{Pe}\frac{dY_{Ng}}{d\bar{r}}\right)_w, \ \bar{h}_l = \left(\frac{Le}{Pe}\frac{d\bar{h}}{d\bar{r}}\right)_w \qquad (16)$$

$$\bar{r} \to \infty : \bar{h} = 1, \ Y_i = Y_{ie} \ for \ i = 1,...,N \qquad (17)$$

Analytical Solution: For analytical solution a new variable [14] is introduced as

$$\xi(\bar{r}) = \int_{\bar{r}}^{+\infty} \frac{Pe}{\bar{r}^2} d\bar{r} \Rightarrow \frac{d}{d\bar{r}} = -\frac{Pe}{\bar{r}^2} \frac{d}{d\xi} \qquad (18)$$

By varying $\bar{r}$ from 1 to ∞, $\xi(\bar{r})$ changes from ξ_w to 0. ξ_w is defined as

$$\xi_w = \int_1^{+\infty} \frac{Pe}{\bar{r}^2} d\bar{r} \qquad (19)$$

Using above variable, Eqs. (14) and (15) are transformed to

$$\frac{dY_i}{d\xi} = \frac{d^2 Y_i}{d\xi^2}, \ i = 1,...,N \qquad (20)$$

$$\frac{d\bar{h}}{d\xi} = -Le \frac{d^2 \bar{h}}{d\xi^2} \qquad (21)$$

Solutions of Eqs. (20) and (21) are:

$$Y_i = A_i + B_i \exp(-\xi(\bar{r})), \ i = 1,...,N \qquad (22)$$

$$\bar{h} = C_1 + C_2 \exp(\frac{-\xi(\bar{r})}{Le}) \qquad (23)$$

Where A_i, B_i, c_1 and c_2 are obtained from boundary conditions.

$$Y_i = Y_{ie} \exp(-\xi(\bar{r})), \ i = 1,...,N-1$$

$$Y_N = 1 - (1 - Y_{Ne})\exp(-\xi(\bar{r}))$$

$$\bar{h} = 1 - \bar{h}_l \exp(\frac{-\xi_w}{Le})(1 - \exp(\frac{-\xi(\bar{r})}{Le})) \qquad (24)$$

The relation between $\bar{r}$ and ξ can be derived from modified Hertz–Knudsen equation for non-equilibrium evaporation [14]. But for simplicity, in constant pressure problems it is assumed that $\rho D = \frac{Const}{\rho}$ [33].

$$\frac{\rho D}{\rho_e D_e} = \frac{\rho_e}{\rho} = \frac{h}{h_e}\frac{R C_{pe}}{C_P R_e} = \frac{\bar{h}(\gamma - 1)}{\gamma}\frac{\gamma_e}{\gamma_e - 1} \qquad (25)$$

Neglecting the γ variations in space lead to

$$\frac{\rho D}{\rho_e D_e} = \bar{h} \qquad (26)$$

According to Eq. (26), Peclet Number can be calculated as

$$Pe = \frac{\dot{m}r_w}{\rho D} = \frac{\dot{m}r_w}{\rho_e D_e} \frac{\rho_e D_e}{\rho D} = \frac{Pe_e}{\bar{h}} \tag{27}$$

Substituting above equation into Eq. (18) yields

$$\frac{d\xi}{d\bar{r}} = -\frac{Pe_e}{\bar{h}\bar{r}^2}, \qquad \xi(\infty) = 0 \tag{28}$$

thus

$$\bar{r} = \frac{Pe_e}{\xi + \bar{h}_l \exp(\frac{-\xi_w}{Le})(Le - \xi - Le \times \exp(\frac{-\xi(\bar{r})}{Le}))} \tag{29}$$

or

$$\xi = LeW \left(\bar{h}_l \exp\left(\frac{\xi_w}{Le}\right) \exp\left(\frac{\dfrac{Le\bar{h}_l\left(Le\bar{h}_l \exp\left(\frac{\xi_w}{Le}\right)\bar{r} - Pe_e\right)}{\left(1 - \bar{h}_l \dfrac{Le\bar{h}_l \exp\left(\frac{\xi_w}{Le}\right)\bar{r} - Pe_e}{\left(1 - \bar{h}_l \exp\left(\frac{\xi_w}{Le}\right)\right)Le\bar{r}}\right)Le\bar{r}}{\left(1 - \bar{h}_l \exp\left(\frac{\xi_w}{Le}\right)\right)Le\bar{r}}\bar{r} - Pe_e}{1 - \bar{h}_l \exp\left(\frac{\xi_w}{Le}\right)} \right) \right)$$

$$- \left(\frac{Le\bar{h}_l \exp\left(\frac{\xi_w}{Le}\right)\bar{r} - Pe_e}{(1 - \bar{h}_l \exp\left(\frac{\xi_w}{Le}\right))\bar{r}} \right) \tag{30}$$

Where W is Lambert function.

Following relation can be evaluated from boundary condition $\xi(1) = \xi_w$

$$Pe_e = (1 - \bar{h}_L \exp(\frac{\xi_w}{Le}))\xi_w + \bar{h}_L Le\left(\exp(\frac{\xi_w}{Le}) - 1 \right) = \xi_W - \frac{\bar{h}_L}{2Le}\xi_w^2 - 0(\xi_w^3) \tag{31}$$

or

$$\xi_w = \frac{Le}{\bar{h}_L}\left(1 - \sqrt{1 - \frac{2\bar{h}_L Pe_e}{Le}} \right) \tag{32}$$

RESULTS

It is assumed that the Freon-11 evaporates into the atmosphere and $\bar{h}_L = 0.54$, $Pe_e = 0.28$ and Y_{ne} are obtained for Freon-11 [14]. The following results show the influence of the Lewis number on the non-equilibrium evaporation.

Variations of the dimensionless specific enthalpy versus dimensionless radius for different values of Lewis number are shown in Fig. 2. By increasing the Lewis number the contribution of thermal diffusion is enhanced. As a result, specific enthalpy is increased, but these variations are more obvious near the droplet surface. For example for Le=0.75, 1, 1.5 and 2 the dimensionless
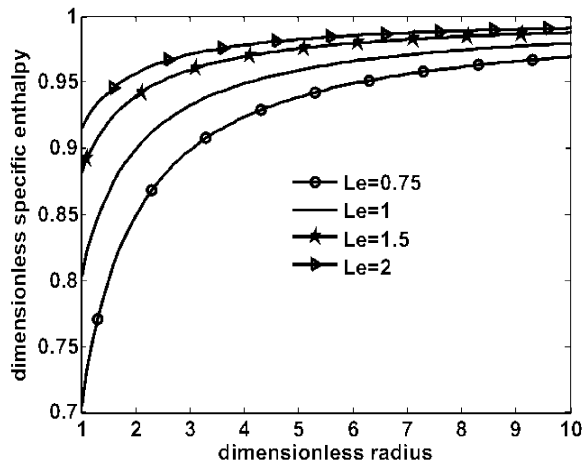
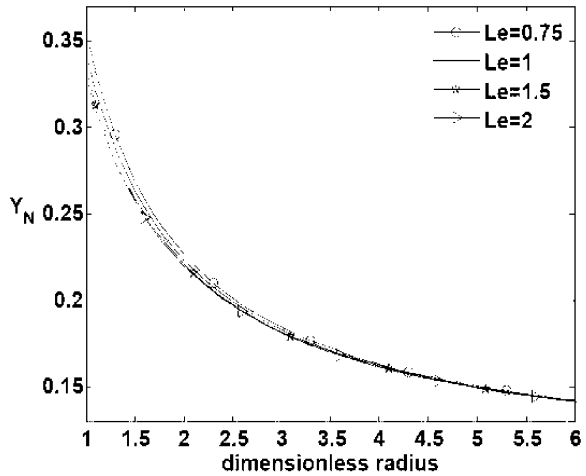Fig. 2: Variations of the dimensionless specific enthalpy versus dimensionless radius for different Lewis numbers
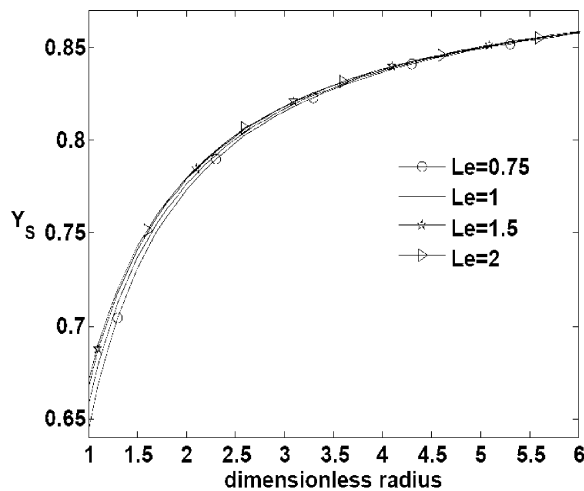

Fig. 3: Variations of mass concentration of the gas surrounding the droplet as a function of dimensionless radius for different values of Lewis number. Y_S is defined as $Y_S = \sum_{i=1}^{N-1} Y_i$

Fig. 4: Effect of Lewis number variations on mass concentration of evaporated Freon-11 as a function of dimensionless radius
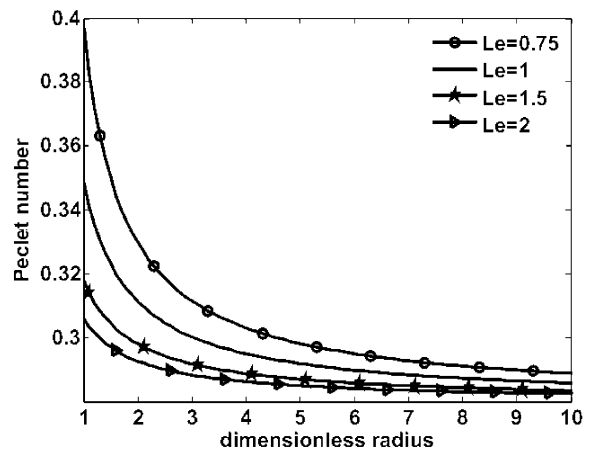

Fig. 5: Variations of Peclet Number versus dimensionless radius for different Lewis numbers
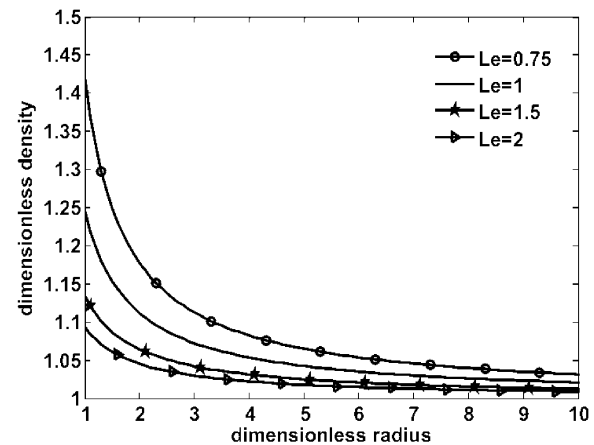
Fig. 6: Variations of dimensionless density as a function of dimensionless radius for different Lewis numbers

specific enthalpy in droplet surface is 0.7052, 0.8035, 0.8814 and 0.9149, respectively.

Figs. 3 and 4 show the variations of mass concentration of the components as a function of dimensionless radius for different values of Lewis number. As it can be seen the variations of the Lewis number has not remarkable effect on the concentration of the components. For instance, as an input Le={0.75, 1, 1.5, 2}, outputs will be: Y_S = {0.6453, 0.6586, 0.6679, 0.6716} and Y_N = {0.3547, 0.3414, 0.3321, 0.3284}, respectively.

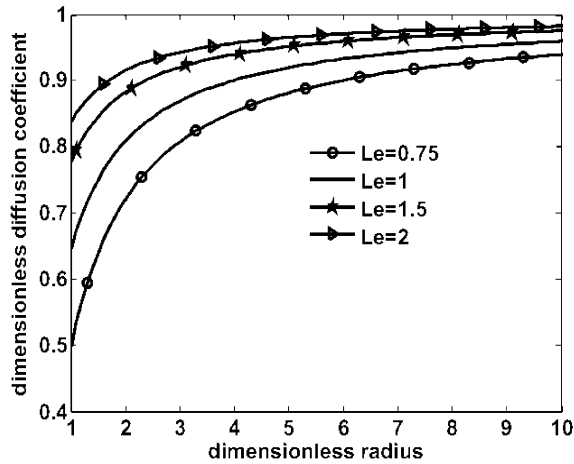Fig. 7: Variations of dimensionless diffusion coefficient versus dimensionless radius for different Lewis numbers

Figs. 5, 6 and 7 show the variations of Peclet Number, dimensionless density and dimensionless diffusion coefficient versus dimensionless radius for different values of Lewis number. By increasing the Lewis number the contribution of thermal diffusion is enhanced. As a result, Peclet Number and density are decreased, whereas diffusion coefficient is increased. These variations are more obvious near the droplet surface as mentioned in Fig. 2.

CONCLUSION

The effects of Lewis number on non-equilibrium droplet evaporation are developed analytically and following results are obtained.

- Lewis number effect on specific enthalpy, Peclet Number, density and diffusion coefficient is stronger than its effect on mass concentration.
- Lewis number is proportional to specific enthalpy, diffusion coefficient and mass concentration of the gas surrounding the droplet, but has an inverse relation with Peclet Number, density and mass concentration of evaporated Freon-11.
- The deviation from equilibrium conditions is large near the droplet surface and will be zero at infinity. By increasing the Lewis number, this deviation is decreased. In other words, the contribution of thermal diffusion is increased by increasing Lewis number. Therefore, this process will be similar to equilibrium.

Nomenclature

c_p	specific heat capacity [J/kg K]
p	pressure [Pa]
P_e	Peclet Number
D	diffusion coefficient [m²/s]
Le	Lewis number
h	Specific enthalpy of the mixture [J/kg]
$\dot{m}$	mass flux [kg/m²s]
v	Velocity [m/s]
r	Spherical radial coordinate [m]
h_L	Latent heat of evaporation [J/kg]
R	Universal gas constant [J/mol K]
T	Temperature [K]
Y	Mass fraction

Greek Symbols

λ	Thermal conductivity [W/m K]
ρ	Density [kg/m³]

Subscripts

I	Species
g	Gas
l	Liquid
e	Infinity
w	Droplet surface

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