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EVALUATION OF DROPLET EVAPORATION MODELS FOR GAS-LIQUID FLOW SIMULATIONS

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Abstract. *Classical droplet evaporation models, including equilibrium and non-equilibrium formulations, that are usually used in spray combustion calculations, are evaluated in this study through comparison of diameter and temperature evolution predictions with experimental data. Furthermore, the effects of ambient pressure variation on the evaporation of a droplet are investigated. The physical model consists of an isolated single-component droplet vaporizing in gas environmental with uniform temperature and pressure, representing an ideal model of the physical phenomena involved in the diluted regions of a spray. Transient droplet heating effects and variable thermophysical properties, for both phases, are considered. The results reveal that, as expected, the non-equilibrium effects are insignificant for the simulated initial diameter, slip velocity and ambient temperature. It is additionally observed that ambient pressure variation from 1 atm to 10 atm does not enhance non-equilibrium effects.*

Keywords: *evaporation, droplet, Lagrangian.*

1. INTRODUCTION

Evaporation of liquid droplets in high temperature gas environment plays an important role in technical applications. In industry, for instance, such phenomenon is observed in furnaces, chemical reactors, gas turbines, internal combustion engines, among others (Jenny *et al*., 2012 and Sazhin, 2006). Due to improper handling, most of these procedures and devices are not operated under optimal conditions. Therefore, understanding the fundamental mechanisms that govern the dynamics of droplet evaporation, as well as breakup, dispersion, mixing and combustion, could improve industrial proceedings, resulting in higher work efficiency and safer operability.

According to Ma (2016), a complete single droplet evaporation model involves simultaneous heat and mass transfer, including, basically, four parts, as presented in Fig.1. These submodels are as follows: Liquid Phase Model (LPM) that considers heating modelling formulation, by assuming the existence of temperature gradient inside the droplet and internal vortical flow; Droplet Surface Properties (DSP) model that enable choosing between equilibrium condition at droplet surface or non-equilibrium state; gas side Heat and Mass Transfer (HMT) model that actually represents droplet mass and temperature variation through time; and Seen Gas Properties (SGP) model that incorporates the effect of reference conditions for thermodynamic and transport properties evaluation.

It is known that when the Classical Evaporation Model (CEM), first reported by Spalding (1953) and Godsave (1953) is adopted as HMT, together with the infinite conductivity approach for LPM, the resulting model typically overpredicts the instantaneous evaporation rate (Jenny *et al*., 2012). As a result, size reduction predictions lead to shorter droplet lifetimes than those observed in experiments. Thus, as an attempt to improve evaporation models, some corrections have already been proposed, such as using a deviation factor for taking into consideration the heat transfer reduction due to evaporation, as in the classical evaporation model (CEM*), and adopting non-equilibrium condition at the droplet surface, as in the non-equilibrium model (NEQ).

The purpose of this study is, therefore, to investigate the consistency of some evaporation models widely used in literature by comparing experimental data predictions with numerical simulations. A n-decane droplet with initial diameter $D_{d,0} = 2.0\ mm$, initial temperature $T_{d,0} = 315\ K$ and Reynolds number $Re_d = 17$, based on a constant slip velocity, is in an air environment with pressure $p_g = 1\ atm$ and $T_g = 1000\ K$, as the experiment made by Wong and

Lin (1992). Hereafter, the ambient pressure is changed to 10 atm to assess how pressure variation affects the evaporation process.

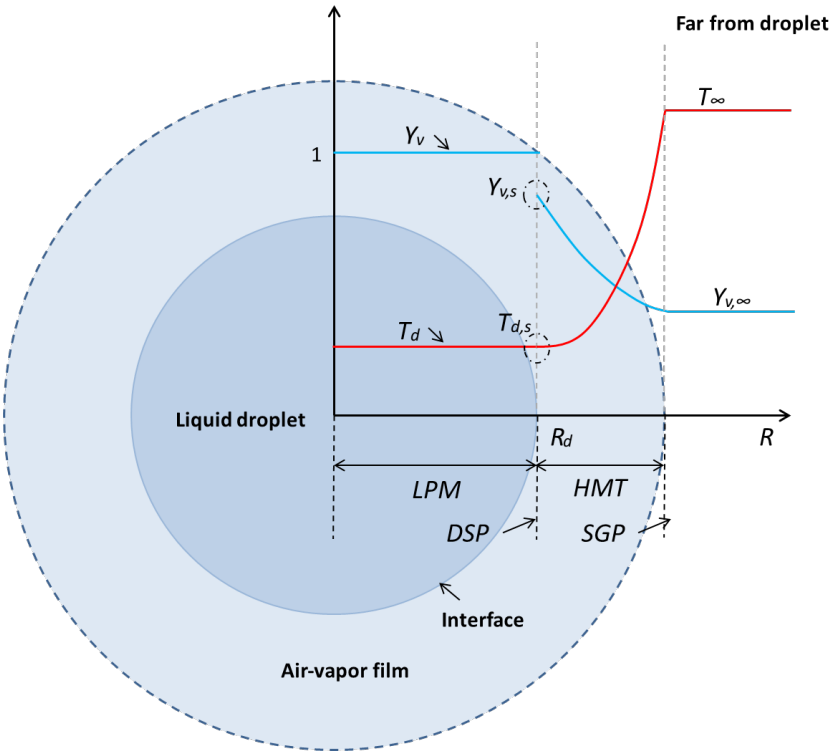

Figure 1: Illustration of the evaporation model division in which the blue line represents the mass fraction profile and the red line represents the temperature profile when uniform temperature is assumed inside the droplet. This figure was adapted from Ma (2016).

2. FORMULATION

Following Miller *et al.* (1998), the generic Lagrangian equations describing droplet mass (m_d) and temperature (T_d) rates of change can be written as Eqs. (1) and (2).

$$\dot{m}_d = \frac{dm_d}{dt} = \frac{-Sh}{3Sc_g}\left(\frac{m_d}{\tau_d}\right) H_M, \tag{1}$$

$$\frac{dT_d}{dt} = f_c \frac{Nu}{3Pr_g}\frac{Cp_g}{Cp_l}\left(\frac{T_g - T_d}{\tau_d}\right) + \frac{L_v}{Cp_l}\frac{\dot{m}_d}{m_d}, \tag{2}$$

where f_c is a correction factor to heat transfer due to evaporation, Nu and Sh are the Nusselt and Sherwood number, Pr_g and Sc_g are the Prandtl and Schmidt number for the gas phase, Cp_g and Cp_l are the specific heat of each phase, T_g is the ambient temperature, L_v is the latent heat of evaporation, H_M represents the specific driving potential for mass transfer due to vapor concentration gradient and τ_d is the particle response time, defined by Eq. (3).

$$\tau_d = \frac{\rho_d D_d^{\,2}}{18\mu_g}, \tag{3}$$

where ρ_d is the droplet density, μ_g is the gas dynamic viscosity and D_d is the droplet diameter.

Since the well-know Frossling correlations overestimate the transfer rate at low Reynolds number, Abramzon and Sirignano (1989) recommend using Eqs. (4) and (5), considering that $1 < Re_d < 400$.

$$Nu = 1 + (1 + Re_d\ Pr_g)^{1/3}\ Re_d^{\ 0.077}, \tag{4}$$

$$Sh = 1 + (1 + Re_d\ Sc_g)^{1/3}\ Re_d^{\ 0.077}. \tag{5}$$

If the thermal energy exchange between phases is assumed to occur only through convective transfer, neglecting radiation effects, and internal droplet vertical flow, as well as temperature gradient, is ignored, LPM considers only an uniform but time-varying droplet temperature, which is known as the infinite-liquid-conductivity model. These considerations can be seen as reasonable approximations considering the small size of the droplets studied.

For DSP both approaches are considered and compared. The key difference between them is the treatment of droplet surface properties; the former uses the equilibrium formulation by Clausius-Clapeyron law, and the latter uses the Langmuir-Knudsen law in order to correct the mole fraction of fuel vapor at the droplet surface, as proposed by Miller *et al.* (1998). As suggested by Sadiki *et al.* (2013). Langmuir-Knudsen law should be used for general gas-liquid flow calculations, because it incorporates realistic non-equilibrium evaporation behavior prevailing in many practical situations, like gas turbine conditions. These considerations are incorporated in the evaporation model by means of the Spalding mass transfer number (B_M).

As shown in Fig. 1, temperature and vapor concentration conditions change abruptly from the droplet surface to the limit of the air-vapor film. As a consequence, a criterion should be chosen to calculate thermodynamic and transport properties of the mixture composition. The most used method is based on the idea of weighting droplet surface and gas properties. The "1/3 rule", suggested by Hubbard *et al.* (1975) and Yuen and Chen (1976), is adopted as SGP to determine references temperature and vapor mass fraction.

As HMT, three different models are selected to be investigated. Basically, the parameters f_c and H_M, from Eqs. (1) and (2), vary from one model to another as shown in Table 1. An analytical expression for heat transfer reduction due to evaporation, G, is incorporated in both models, equilibrium and non-equilibrium, to check its performance. This expression, showed in Eq. (6), was first obtained in El Wakil *et al.* (1954). As observed by Miller *et al.* (1998), for non-evaporating droplets analysis, $G \to 1$ as $\beta \to 0$.

$$G = \frac{\beta}{e^{\beta} - 1}, \tag{6}$$

where β is defined by Eq. (7).

$$\beta = -\left(\frac{3Pr_g\,\tau_d}{2}\right)\frac{\dot{m}_d}{m_d}. \tag{7}$$

Table 1. Expressions for the evaporation correction factor and mass transfer potential.

Model	*Name*	f_c	H_M
CEM	Stefan-Maxwell	1	ln (1+$B_{M,eq}$)
CEM*	Modified Stefan-Fuchs	G	ln (1+$B_{M,eq}$)
NEQ	Langmuir-Knudsen	G	ln (1+$B_{M,neq}$)

3. RESULTS AND DISCUSSION

Figures 2(a)-(d) show the temporary variation of the non-dimensional droplet diameter squared, $(D_d/D_{d,0})^2$, the droplet temperature, vaporization rate $(\dot{m}/m_0)$ and Lewis number (Le), respectively. Figures 2(a) and (b) are compared with experimental data from Wong and Lin (1992), evidencing that the relatively large difference between ambient temperature and initial droplet temperature results in a strong initial heat up transient stage during which the "D^2 law" is not obeyed. Also, as expected, after a first increase, the droplet temperature reaches an equilibrium or wet-bulb temperature (Abramzon and Sazhin, 2005). At that temperature, all of the heat coming to the droplet surface from the gas is spent on evaporation; as a result, the sensible heat penetrating to the liquid phase becomes zero. Figure 2(c) confirms that the CEM overpredicts the instantaneous vaporization rate, resulting in poor representation of droplet diameter and temperature temporal evolution.

As stated in Sacomano *et al.* (2017), the Lewis number is computed at each time step based on the thermodynamic and transport properties evaluated at the air-vapor film with the "1/3 rule". Thus, the unitary Le assumption is not applied in the droplet surrounding film. Figure 2(d) indicates that $Le \rightarrow 1$ for CEM as assumed in most situations for the carrier phase; however, for CEM* and NEQ, models whose results seem to be more valid when compared with experimental data, $Le \rightarrow 1.5$. It is important to note that if $Le = 1$, it means that thermal and mass diffusivities are equal, which is not a reasonable assumption for evaporation of fuel droplets.

Figures 3(a)-(c) confirm the behavior described by Chrigui *et al.* (2012) when the non-equilibrium effects are taken into account. That is, the surface vapor mass fraction decreases, causing the reduction of the Spalding mass transfer number and, consequently, there is an augmentation of the Sherwood number. Nevertheless, this tendency is also observed in the CEM* results, that neglects non-equilibrium effects.

From Figs. 2 and 3, it can be noted that CEM* and NEQ predictions are similar, demonstrating that, for the conditions of the tested case, only the heat transfer correction for evaporation, incorporated by f_c, influences the simulated results. Hence, the term that corrects molar fraction of fuel vapor at droplet surface makes no difference, not even in the end of the droplet lifetime.

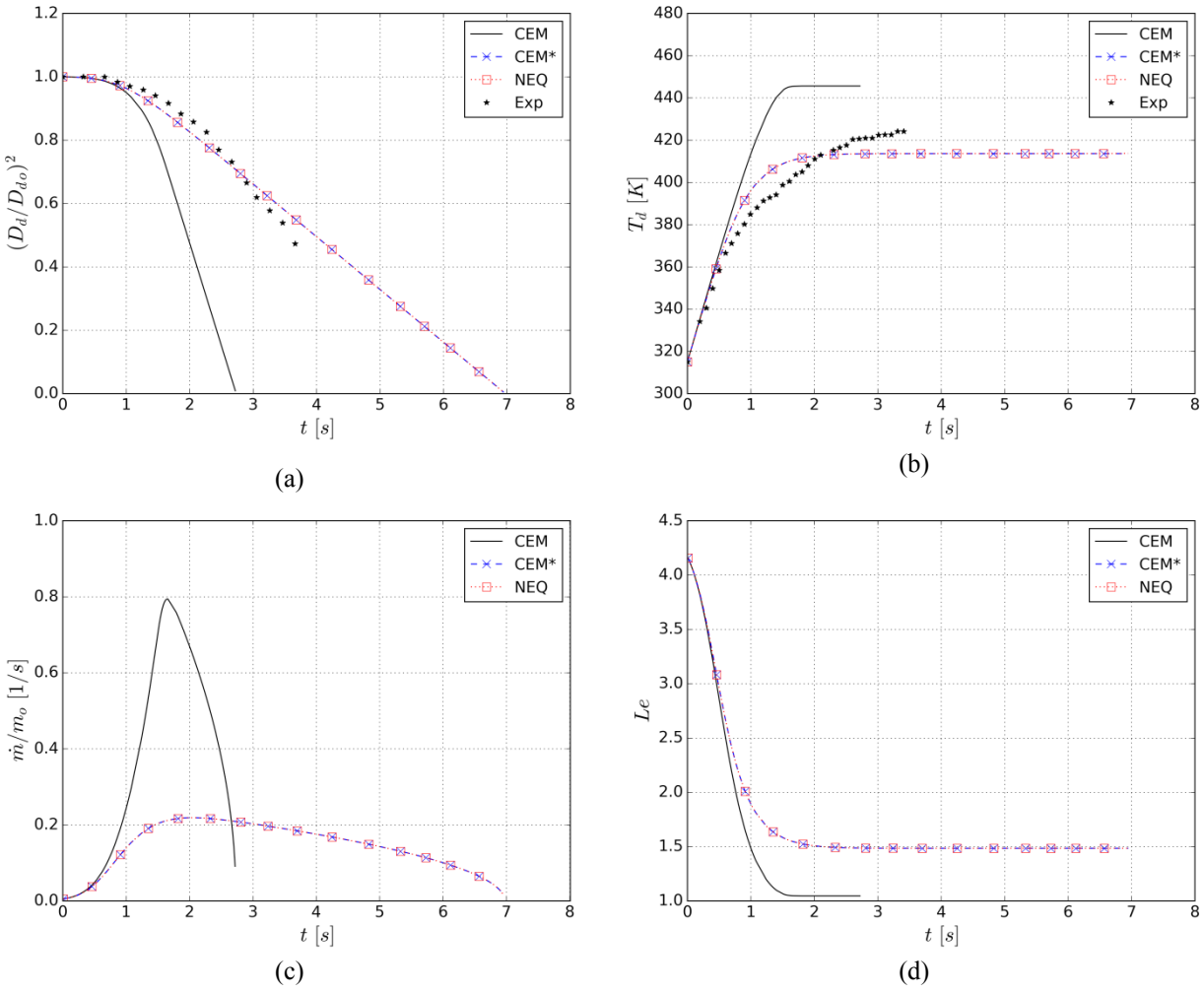

Figure 2: Temporal evolution of (a) non-dimensional droplet diameter squared; (b) droplet temperature; (c) vaporization rate; and (d) Lewis number for ambient pressure of 1 atm.

Comparing Figs. 2(a) and (b) with Figs. 4(a) and (b), it is observed that once the ambient pressure increases, the ratio of initial heat up time to the whole evaporation lifetime increases, making the non-dimensional droplet diameter squared curve becomes more round in the beginning. These observations were reported by Nomura *et al.* (1996) as a conclusion based on their experimental study with n-heptane droplets. For ambient pressure of 10 atm, the droplet temperature also achieves a plateau approximately in the wet-bulb temperature. Furthermore, it is observed that ambient pressure variation from 1 atm to 10 atm does not enhance non-equilibrium effects, since CEM* and NEQ curves are still similar.

4. CONCLUSIONS

It can be concluded that the conditions of the simulated case, which are based on available experimental data, do not satisfy the criteria necessary to be influenced by non-equilibrium effects. Miller *et al.* (1998) suggested that the non-equilibrium effects only influence droplet diameter and temperature predictions when the initial droplet diameter is small enough. Besides that, their results also reveal that thermodynamic non-equilibrium effects could be important depending on ambient temperature and slip velocity. To the best of the authors' knowledge, there are not available experimental measurements for single droplets with initial diameter smaller than 50 μm in the literature.

Notwithstanding spray combustion applications usually have droplets diameter smaller than 50 μm, there are experimental limitations concerning initial droplet diameter. The difficulties in measuring the droplet size and surface temperature and the inherent errors in the measuring equipment may deteriorate the accuracy of the experimental data.

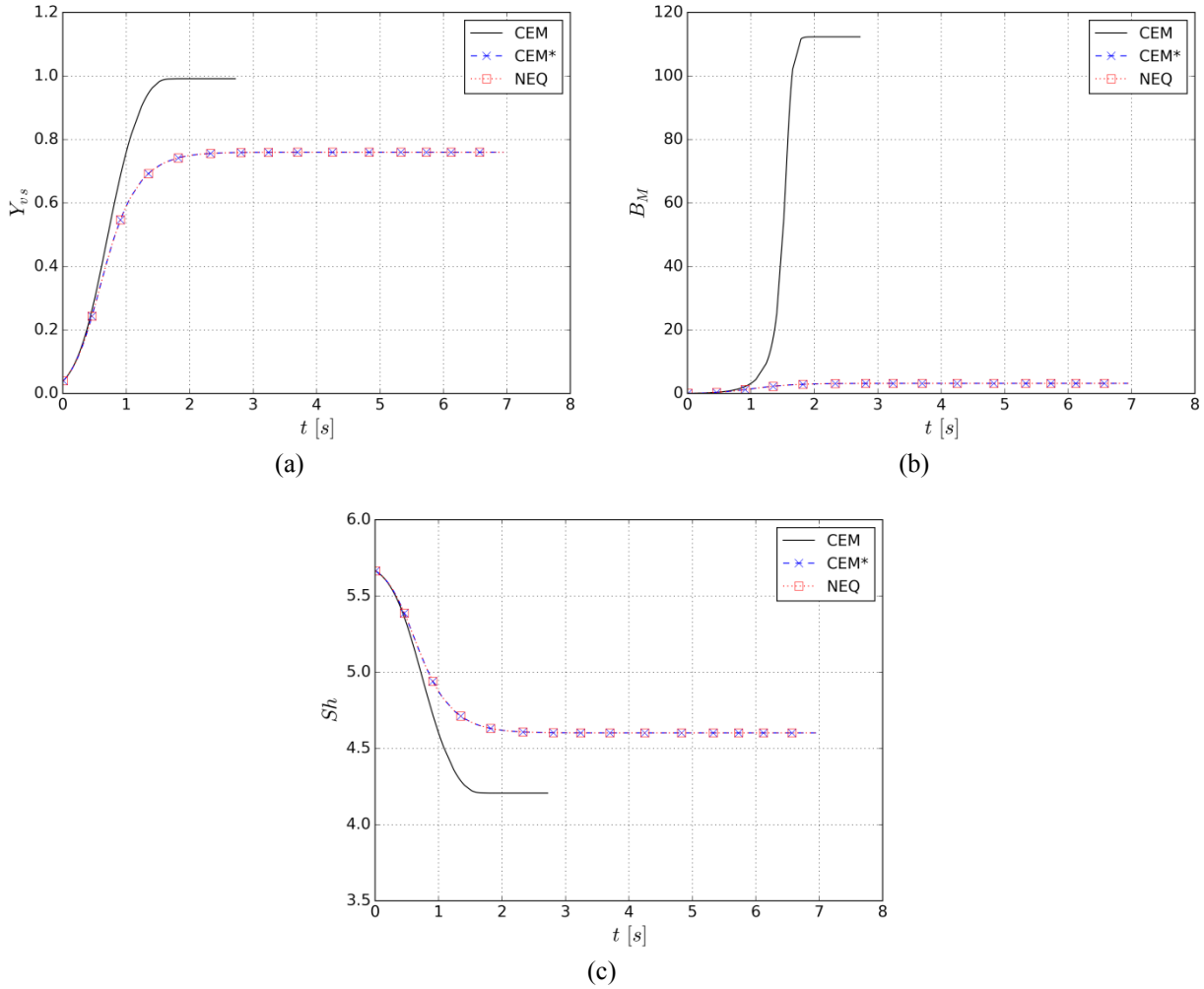

Figure 3: Temporal evolution of (a) mass fraction of fuel vapor at droplet surface; (b) Spalding mass transfer number; and (c) Sherwood number for ambient pressure of 1 atm.

Despite the conclusions drawn in this study, there are still some open questions about the applicability of these models for spray simulations that needs to be carefully analyzed with particular emphasis on computational cost for a large number of droplets. For spray combustion applications, the effects of interaction between droplets and how turbulence effects influence the evaporation process should also be investigated.

5. ACKNOWLEDGEMENTS

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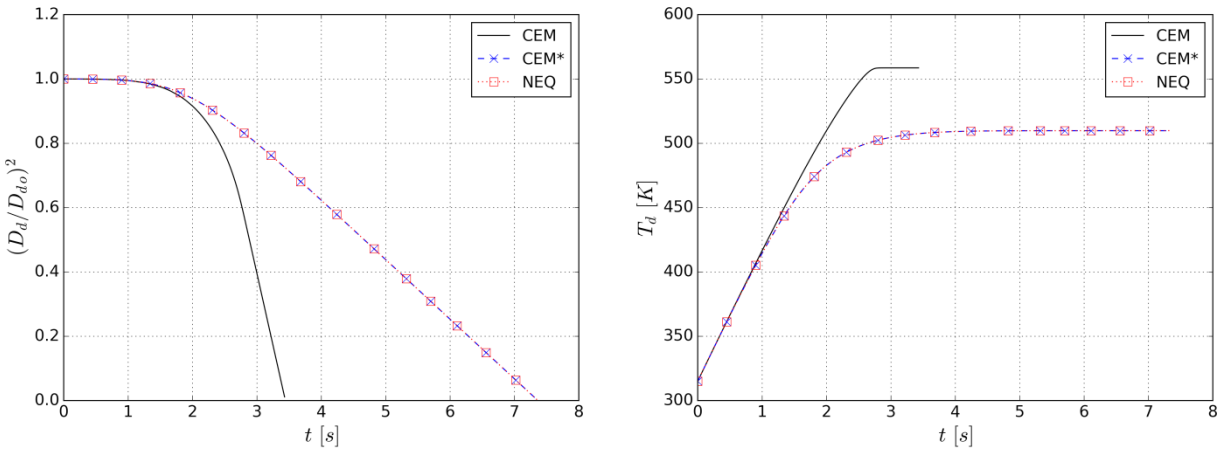

(a) (b)

Figure 4: Temporal evolution of (a) non-dimensional droplet diameter squared and (b) droplet temperature for ambient pressure of 10 atm.

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