



Transient temperature gradient in a single-component vaporizing droplet



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ABSTRACT

The purpose of this work is to analyze the importance of considering internal temperature non-uniformity in modeling droplet evaporation, and to demonstrate performance of simplified methods in which the temperature gradient is approximately taken into account. Based on three characteristic time scales, two dimensionless criteria are identified which determine magnitude of the internal temperature gradient and its effect on the evaporation dynamics. Numerical values of these criteria in a wide range of ambient temperatures show that the effect of the internal temperature gradient is more pronounced in a more volatile liquid at higher ambient temperatures. Although droplet life time predictions are not sensitive to the internal temperature gradient, its effect might be considerable at the initial stages of droplet evaporation, and this substantiates the need in robust and computationally inexpensive methods to take it into account. Three simple and yet accurate approaches (the power law approximation, the higher order polynomial approximation and the integral heat balance method) have been favorably tested and recommended for use in CFD spray modeling.

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1. Introduction

Adequate prediction of droplet heating and evaporation is a key component of turbulent spray modeling in studies of liquid fuel injection, fire suppression, among many other engineering applications and environmental phenomena. In all these cases, a very large amount of droplets should be considered. Therefore, simplified models for transport of mass and energy both in gas and liquid phases are required. For a single droplet, gas phase models are based on analytical solutions of the vapor mass and energy conservation equations [1,2]. These solutions are obtained assuming spherical symmetry and produce explicit expressions for droplet evaporation rate. Convective flow around the droplet is then approximately taken into account by introducing Sherwood and Nusselt numbers which are estimated from the empirical correlations depending on flow Reynolds number as well as Schmidt and Prandtl numbers. The latter correlations are usually corrected to allow for liquid evaporation. Liquid phase models include overall heat balance of the evaporating droplet which is formulated in terms of volume-average droplet temperature. Meanwhile, the evaporation rate is determined by the surface temperature which may differ from the volume-average one when a considerable internal temperature gradient develops. Nevertheless, in spray modeling it is conventional to assume uniform temperature distri-

bution inside the droplet. It immediately implies that the droplet surface temperature (which solely affects evaporation rate), is assumed to be equal to volume average temperature (which is determined from the heat balance).

Although uniformity of liquid temperature inside a vaporizing droplet (the infinite conductivity concept) is conventionally assumed in most of the existing spray models, its limitations were highlighted in a number of papers, e.g. Law and Sirignano [3], Sirignano [4], Aggarwal et al. [5], Bertoli and Migliaccio [6], Sazhin et al. [7] among others. In the above works, an observable difference has been demonstrated in evaporation rates predicted by assuming finite and infinite liquid conductivity. Such a difference was observed at the initial transient stage of droplet heating in a hot gas environment. It has been recognized that consideration of heat transfer inside the droplet is closely coupled with liquid circulation driven by the shear stress developing at the surface of moving droplet.

Direct resolution of temperature field in a circulating liquid requires numerical solving of at least 2D Navier–Stokes equations in every droplet which is not affordable in spray modeling. An approximate solution to this problem can be obtained using the effective conductivity model in which liquid circulation is accounted for by appropriately increased thermal conductivity of the liquid. Such an effective thermal conductivity is set to be a function of liquid Peclet number which is formulated in terms of estimated liquid velocity at the droplet surface [8]. Within the framework of the effective conductivity concept, the internal heat

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Nomenclature

Latin symbols

a	thermal diffusivity [m^2/s]
\mathbb{B}	evaporation modified Biot number [-]
Bi	Biot number [-]
B_M	mass Spalding number [-]
B_T	thermal Spalding number [-]
c	specific heat [$\text{J}/(\text{kg K})$]
c_0, c_2, c_p	polynomial coefficients [K]
C_D	drag coefficient [-]
C_F	friction coefficient [-]
d	droplet diameter [m]
\mathcal{D}_{vap}	vapor diffusion coefficient [m^2/s]
Fo	Fourier number [-]
g	gravity acceleration [m/s^2]
M	molar weight [kg/mol]
Nu	Nusselt number [-]
Pe	Peclet number [-]
Pr	Prandtl number [-]
q	heat flux [W/m^2]
Q	heat flow [W]
Q_d	net heat flux received by the droplet [W]
Δh_{vap}	enthalpy of vaporization [J/kg]
r	radial coordinate [-]
R	droplet radius [m]
\mathcal{R}	universal gas constant [$\text{J}/(\text{mol K})$]
Re	Reynolds number [-]
\mathcal{S}	thermal non-equilibrium ratio [-]
Sh	Sherwood number [-]
T	temperature [K]
V	droplet velocity relative to gas [m/s]

Y mass fraction [-]

Greek symbols

δ	thermal layer thickness [m]
γ_n	n -th eigenvalue [-]
λ	thermal conductivity [$\text{W}/(\text{m K})$]
ρ	density [kg/m^3]
τ	time scale [s]

Subscripts

<i>air</i>	air
<i>boil</i>	boiling
<i>c</i>	center
<i>conv</i>	convective
<i>d</i>	droplet
<i>eq</i>	equilibrium
<i>eff</i>	effective
<i>g</i>	gas
<i>l</i>	liquid
<i>s</i>	surface
<i>T</i>	temperature
<i>vap</i>	vapor, vaporization
<i>V</i>	velocity
<i>wb</i>	wet bulb
<i>0</i>	initial, ambient

Superscripts

<i>ref</i>	reference value
overbar	volume averaging

transfer model is reduced to the heat conductivity equation only, which can be efficiently solved numerically [13] or treated analytically [2,7,17]. Despite of this, exact (numerical or analytical) solution to this equation in every droplet imposes significant and hardly affordable computational cost, which becomes prohibitive for high-resolution LES.

Therefore, several attempts have been made to develop approximate models which take temperature non-uniformity in vaporizing droplets into account. To allow for the internal heat and mass transfer inside evaporating droplet, an approximate model has been developed by Renksizbulut et al. [9] who described droplet temperature field by two values of surface temperature and droplet core temperature. It was further assumed that due to the heat transfer the difference between these quantities is proportional to the heat flux accepted by the droplet at its surface. The above assumption is equivalent to setting the Nusselt-like number, $q_s R / \lambda_{l,eff} (\bar{T} - T_s)$, calculated at the liquid side of the droplet surface to be constant. In fact, this assumption is a consequence of establishing quasi-steady temperature field inside the droplet, and this is clearly illustrated using the quasi-steady parabolic approximation (see Eq. (26), which shows that $q_s R / \lambda_{l,eff} (\bar{T} - T_s) = 1/5$). Not surprisingly, such an approximation is not valid at early times of droplet heating (or cooling); this issue is discussed in detail in this paper.

Two-temperature approach can be derived more rigorously if a particular functional form of internal temperature distribution is assumed. This is the idea of parabolic approximation when the radial temperature distribution is assumed to be second order polynomial as suggested by Dombrowsky and Sazhin [10]. The droplet

core temperature is formally defined as volume-averaged temperature which is coupled (via heat balance ODE) to droplet surface temperature and the heat flux received by the liquid. Note, that approximation of this type was earlier used for modeling diffusion of lithium particles of active material, e.g. by Subramanian et al. [11]. A more elaborate approach was proposed by Zeng and Lee [12], who constructed a first order differential equation (see Eq. (34)) to model relaxation of the difference between the surface and volume-averaged temperatures $T_s - \bar{T}$ to the equilibrium value of $-(Rq_s / \lambda_{l,eff})/5$, corresponding to the parabolic profile. More recently, two-temperature approach was applied in the model by Balasubramanyam et al. [14]. However, instead of using constant value for the proportionality coefficient between the surface and core temperatures, this coefficient was calculated by Balasubramanyam et al. [14] from thermal resistance of thermal boundary layer with effective thermal diffusivity, a_{eff} , estimated for (presumably) fully developed turbulent liquid flow inside the droplet. Thickness of the thermal boundary layer was calculated as $\sqrt{\pi a_{eff} \Delta t}$, which is questionable when its value is comparable to the droplet radius. Furthermore, the time scale, Δt , is set equal to the evaporation sub-cycle time step which introduced another source of a possible inaccuracy to the model. Nevertheless, such a model was successfully applied by Balasubramanyam and Chen [15] to predict evaporating spray penetration in a high-speed cross-flow. Use of the above finite-conductivity model improved agreement of the predictions with the measurements, although its effect appeared to be comparable to (or even weaker than) the effect of the error introduced by the drag coefficient. It is difficult to extend this conclusion to other conditions of spray

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