An Investigation of Liquid Droplet Evaporation Model Used in Multiphase Flow Simulation

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ABSTRACT
Modeling liquid droplet evaporation in a flow stream is very important in many engineering applications. It was discovered that the result of predicted droplet and main flow temperatures from using commercial codes sometimes presents unexplainable phenomena; for example, the droplet temperature drops too low. The objective of this study is to investigate the issues involved in the built-in droplet evaporation model by using three different approaches: (a) use the existing built-in correlations model in a commercial code, (b) use the lumped analytical analysis, and (c) actually solve the heat and mass transfer by directly using CFD without employing the built-in correlation model. In the third approach, the evaporation process is simulated by imposing water evaporation in a very thin layer at the surface of a stagnant water droplet; in the meantime, the evaporation energy is subtracted from the same place. This is performed by imposing a positive mass source term and a negative energy source term in a thin layer of cells wrapping around the droplet surface. The transport equations are then solved using the commercial CFD solver Ansys/Fluent to track the mass and energy transfer across the shell sides into the liquid droplet and out to the ambient. Unlike the built-in evaporation model in commercial codes, which assumes that all the evaporation energy (latent heat) is supplied by the droplet, in the direct CFD calculation, the evaporation energy is absorbed partly from the droplet and partly from the surrounding air according to the natural process based on the property values and the heat and mass transfer resistance inside and outside the droplet. The direct CFD result (without using evaporation correlation) is consistent with that of the lumped analytical analysis (2nd approach). During the development of the direct CFD calculation, several technical difficulties are overcome and discussed in detail in this paper. A revised equation is proposed to improve the existing built-in model in the current commercial code. Both the direct CFD method and the zero-dimensional lumped method show the droplet temperature always increases.

NOMENCLATURE
A Area [m²]
Bi Biot number [hL_/K_s]
C_D Drag Coefficient
C Vapor concentration [kg/m³], Specific heat [J/kg.K].
D, d Diameter [m], Mass diffusion coefficient [m²/s].
E Total energy [J/kg]
h Convective heat transfer coefficient [W/m².K]
h_L Latent heat [J/kg]
K Thermal conductivity, [W/m.K].
K_M Mass transfer coefficient [m/s].
L Length, [m].
m Mass, [kg]
Nu Nusselt number [hL_/K_s]
R_Cond Conduction Resistance [L_s/K_s]
R_Conv Convection Resistance, [1/hA]
Re Reynolds numbers

Greek Letters
µ Absolute viscosity, [Pa.s].
τ Shear stress, [N/m²].
Time scale, [s].

Subscripts:
f Fluid
I Inlet, term number, tensor index (1, 2, 3).
J, k Term number, tensor index (1, 2, 3).
∞ Carrier phase (away from the droplet surface)

INTRODUCTION
The evaporation of liquid droplets in a flow stream is of interest in many fields of engineering such as liquid fuel spray in a combustor, water spray cooling, gas turbine inlet fogging, mist cooling, etc.

The evaporation of liquid droplets has been studied extensively both numerically and experimentally. As known, numerical simulation, if reasonably validated, provides a fast and a cost effective tool to add the experimental studies. Numerous studies have shown the usefulness of using CFD as a tool to predict the evaporation process. Either commercial or
homemade codes have helped to perform that task and have provided enlightened interpretations for the embedded physics of the evaporation process. Occasionally, some glitches appear from using the built-in evaporation models in some commercial CFD codes. For instance, in using one of the commercial codes to calculate liquid droplet evaporation, sometimes the water droplet temperature temporarily reduces significantly and sometimes even below the freezing point during a constant pressure evaporation process. Of course, this cannot happen at a constant-pressure evaporation process because, typically, the droplet temperature should not drop below the wet-bulb temperature. These findings motivate this study to investigate the built-in evaporation models used in some commercial codes.

Classical droplet evaporation theory was developed in the 1950’s by Spalding [1], which yielded the well-known $d^2$-law [2]. In real engineering applications, as in liquid fuel combustion, the collective behavior of clouds of droplets is of great interest. Sprays, created by atomizing liquid fuels, have been considered one of the most efficient ways of burning liquids. The reason for this is that, in a spray, the surface-to-volume ratio is increased greatly compared with a blob of liquid. The extra surface increases the efficiency of heat transport to the liquid, thereby promoting evaporation, ignition, and combustion of the fuel. Of course, the behavior of droplets in a spray is different from that of isolated droplets because of the interaction between droplets and each other and the interactions between drops and the surrounding gases. According to the degree of interaction, the droplet behavior in a spray differs from that of isolated droplets. However, the thermal-flow transport of multiple droplets is more complicated and difficult than that of a single droplet; thus, when the literature review is conducted, it is logical to see that studies of a single isolated droplet were first conducted, followed by relating the single droplet evaporation mechanisms to dilute sprays and drop clouds.

The evaporation of isolated droplets in a stagnant air was studied by Law [3-4]. He proposed a diffusion limit model, taking into account droplet transient conduction and giving an accurate representation of single droplet evaporation in a stagnant environment. However, this model for a stagnant ambiance is inadequate for the convective droplet vaporization. The empirical correlations of the convective single droplet vaporization were formulated by Frossling [5] and Ranz and Marshall [6-7]. Their study on pure liquid droplets confirmed the analogy between heat and mass transfer at low Reynolds numbers. Independent correlations for heat and mass transfer were obtained from the experiments and these empirical correlations have been popular and widely used in most of engineering applications. Refai Ahmed, G. et. al [8] presented an approximate analytical model for predicting forced convection heat transfer from stationery isothermal spheres. Waheed, et al. [9] performed numerical simulations of the mass-transfer of droplets in a continuous phase for a combined-mode problem involving both free- and forced-convections. The effect of free and forced convection on the mass transfer was investigated by solving the complete Navier-Stokes and the convection–diffusion equations using the finite element method. The results showed that superposition of free convection on forced convection didn’t enhance mass transfer.

Smolik and Vitovec [10] numerically analyzed the quasistationary evaporation of a water droplet into a multicomponent gaseous mixture containing a heavier component besides air. The results demonstrated the possibility of condensation of the heavier component on the surface of evaporating droplet as a result of supersaturation. Ferron and Soderholm [11] estimated numerically the evaporation time of a pure water droplet in air with a well defined temperature and relative humidity. Their results, approximated by an equation, showed that the droplet evaporation time is primarily a function of the initial droplet diameter and the relative humidity. Then, Miller et al. [12] evaluated a variety of liquid droplet evaporation models.

High evaporation rates generate a non-uniform temperature distribution at the surface. This creates a surface tension gradient that produces a forcing in which surface fluid is pulled toward regions of higher surface tension. The viscous force then transports momentum into the interior of the droplet and a convective flow results throughout the droplet. This surface-tension-driven instability flow is called the Marangoni instability [13]. A moving surface should also drive convection exterior to the droplet increasing the exterior mass and heat transport. This increased heat and mass transport should increase the evaporation rate. On the other hand, the convection should also tend to equilibrate the temperature at the surface decreasing any surface tension gradients and, therefore, should tend to reduce the convection.

Spells [14] revealed experimentally the circulation patterns in drops of glycerine falling in castor oil and hence subjected to shearing force across its surface. Hegseth et al. [15] have experimentally shown that when a droplet evaporates quickly enough, it exhibits a vigorous interior flow. This flow is driven by surface tension gradients resulting from the non-uniform temperature distribution at the surface.

Unsteady droplet vaporization with slip and an internal circulation has been studied analytically and experimentally by Prakash and Sirignano [16]. They studied in detail the vaporization of fuel droplets flowing with high Reynolds number through a stagnant gas. Similarly, the unsteady investigations of vaporizing hydrocarbon droplets were studied by Dwyer and Sanders [17]. It was assumed that the droplet was always at the boiling point; therefore, the initial liquid heat-up process was not studied. The effects of the internal circulation were neglected.

Regarding the evaporation of a droplet in a cloud of droplets, Milburn [18] had studied the mass and heat transfer process within finite clouds of water droplets. He developed a simple nonlinear differential equation to govern the propagation of vapor concentration, temperature, and droplet size in space and time. Kouska et al. [19] solved the modified Maxwell equation for droplet clouds to evaluate the evaporation rate of mono-disperse water droplets. When the concentration of droplet clouds is sufficiently low, the results of the numerical calculation for droplet clouds agree well with those of a single water droplet. The equilibrated system, where a water droplet cloud is steadily mixed with unsaturated air, was also analyzed.
PROBLEM STATEMENT AND HYPOTHESIS
As mentioned earlier, the problem which motivated this study was originated from the observation during the application of a commercial code to calculate liquid droplet evaporation that, sometimes, the water droplet temperature temporarily reduces significantly below the wet-bulb temperature and sometimes even below the freezing point during a constant pressure evaporation process. As the problem occurred during the droplet evaporation process, it was speculated that the built-in droplet evaporation model might have a problem. The first approach is to examine the fundamental physics involved in the droplet evaporation process. As the droplet evaporates, the surface water molecules need some energy to depart from the surface and change into the vapor phase. This energy is the latent heat of vaporization; but the question remains as to where this energy is coming from. It is hypothesized that the energy is transferred from the surrounding gas, as well as from the droplet itself. Therefore, the relative amount of heat coming from outside and inside the droplet should be weighted according to the differences in the thermal resistances of the heat transfer paths outside and inside the droplet, respectively. These relative proportions of the thermal resistances outside the droplet (convection) and inside the droplet (conduction) are determined with the evaluation of the Biot number. Hence, the droplet evaporation model should reflect the fundamental physics of liquid evaporation by including the mechanism of absorbing latent heat from both the surrounding gas, as well as from the droplet itself as controlled by the Biot number.

The current work starts with conducting a fundamental study of water droplet evaporation models and physical processes. It eventually aims at modifying the current built-in evaporation models in an existing commercial CFD code. The following approaches are taken sequentially in this study.

(a) Use Ansys/Fluent CFD code with existing built-in evaporation model and associated empirical correlations to study the evaporation process of water droplets.
(b) Use a simple zero-dimensional lump-capacitance model to analyze the problem and modify the droplet evaporation energy equation.
(c) Solve the heat and mass transfer of a single droplet during evaporation by directly using CFD without employing the built-in model. This provides an opportunity to understand the physics of the droplet evaporation process in depth and verify the hypothesis proposed in this study. (Note: This is not the direct numerical simulation, or DNS.)

(I) CFD CALCULATIONS USING BUILT-IN EVAPORATION MODEL
In this approach, the existing evaporation model available in Ansys/Fluent CFD code is used. A feasible method to simulate the evaporation of water droplets is to consider the droplets as a discrete phase since the volume fraction of the liquid is small (less than 0.1%). The trajectories of the dispersed phase (droplets) are calculated by the Lagrangian method (Discrete Phase Model, DPM). The impacts of the droplets on the continuous phase are considered as source terms to the governing equations of mass, momentum, energy, and species. The discrete phase model (DPM) along with the standard evaporation model is used.

The Computational Domain
The computational domain is a 2D duct (0.4 m ×3 m). The droplets are injected as a group of 4 streams equally spaced at the inlet. The ratio of the mass flow rate of the injected water to the air mass flow rate has been chosen to be small (1 × 10^6). This ensures that the droplet-droplet interaction effects can be neglected and makes the assumption of isolated droplet reasonable.

Mathematical Model for the Carrier Phase
Air, which is the carrier (continuous) phase, is treated as a perfect gas mixture composed of two species: air and water vapor. The governing equations include conservation of mass, conservation of momentum, conservation of energy, and conservation of species. In addition to these governing equations, other auxiliary equations are used to calculate the density, viscosity, and thermal conductivity for the mixture.

Governing equations
Since the droplet Reynolds number, based on the slip velocity, is approximately 3, laminar flow is assumed. The following are the governing equations of mass, species, momentum, and energy for unsteady laminar flow conditions.

\[
\frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}(pu_i) = S_m \\
\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}(\tau_{ij}) + S_f \\
\frac{\partial (\rho c_p T)}{\partial t} + \frac{\partial}{\partial x_i}(\rho c_p u_i T) = \frac{\partial}{\partial x_i}(\lambda \frac{\partial T}{\partial x_i}) + \mu \Phi + S_h \\
\frac{\partial \rho Y_j}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_j) = \frac{\partial}{\partial x_i}(\rho D_j \frac{\partial Y_j}{\partial x_i}) + S_j
\]

where \(\tau_{ij}\) is the symmetric stress tensor. The source terms \((S_m, S_p, S_h, S_h)\) are used to include the contributions of the droplet evaporating species, droplet forces, and evaporation energy from the dispersed phase (water droplets). During evaporation, water vapor diffuses and is convected into the surrounding gas through the species transport equation, Eq. 4. Here \(Y_j\) is the mass fraction of species \(j\) in the mixture; \(S_j\) is the source term of species; and \(D_j\) is the diffusion coefficient.

Discrete Phase Model (Water Droplets).
As the injected water mass flow is very small and the droplet diameter is also small, the volume fraction of water droplet to air is expected to be small (<10 %), which is the sufficient condition to use the DPM. Following the governing equations for the droplet flow:

Droplet Flow and Heat Transfer- The droplets are tracked by Lagrangian method by applying Newton’s 2nd Law with the following equation of motion

\[
m_p \frac{dV_p}{dt} = \sum F = F_D + F_g + F_{th} + F_S
\]

where \(m_p\) is the droplet mass, and \(V_p\) is the droplet velocity (vector). The right-hand side is the combined force acting on the droplets, including \(F_D\) (drag force), \(F_g\) (gravity and
buoyancy force), $F_S$ (Saffman lift force) and $F_{th}$ (thermophoretic force). For more details about these forces see [20].

The droplet temperature change depends on convection, evaporation, and radiation. The energy equation for any individual droplet can be given as the following equation:

$$m_c c_p \frac{dT}{dt} = \pi d^2 h(T_{\infty} - T) + \frac{dm_p}{dt} h_{fg} + \text{Radiation} \tag{6}$$

where $h_{fg}$ is the latent heat. The radiation heat transfer term can be reasonably neglected because the range of temperatures is low in this study.

The convective heat transfer coefficient ($h$) can be obtained with an empirical correlation [6-7] as follows:

$$\text{Nu}_d = \frac{h_d}{\lambda} = 2.0 + 0.6 \text{Re}^{0.5} \text{Pr}^{0.33} \tag{7}$$

where $\text{Nu}$ is the Nusselt number, and $\text{Pr}$ is the Prandtl number.

The evaporated mass is calculated by two modes: evaporation and boiling. During the evaporation mode, the evaporated mass change rate or vaporization rate is affected by the relative humidity in the air and is shown in Eq. (8) as being governed by the concentration difference between droplet surface and the air stream,

$$-\frac{dm_p}{dt} = \pi d^2 k_c(C_s - C_{\infty}) \tag{8}$$

where $k_c$ is the mass transfer coefficient and $C_s$ is the vapor concentration at the droplet surface, which is evaluated by assuming that the flow over the surface is saturated. $C_{\infty}$ is the vapor concentration of the bulk flow, which is obtained by solving the transport equation in the computational cell. The value of $k_c$ can be given from a correlation analogous to Eq. (7) [6-7] as follows:

$$\text{Sh}_d = \frac{k_d D}{D} = 2.0 + 0.6 \text{Re}^{0.5} \text{Sc}^{0.33} \tag{9}$$

where $\text{Sh}$ is the Sherwood number, $\text{Sc}$ is the Schmidt number (defined as $v/D$), and $D$ is the mass diffusion coefficient of the water vapor in the bulk flow.

When the droplet temperature reaches the boiling point, the following equation can be used to evaluate its evaporation rate [21]:

$$-\frac{dm_p}{dt} = \pi d^2 \left(\frac{\lambda}{D}\right)(2.0 + 0.46 \text{Re}^{0.5}) + \ln(1 + c_p(T_{\infty} - T)/h_{fg})/c_p \tag{10}$$

where $\lambda$ is the gas/air heat conductivity and $c_p$ is the specific heat of the bulk flow.

Theoretically, evaporation can occur at two stages: (a) when the temperature is higher than the saturation temperature (based on local water vapor concentration), water evaporates according to Eq. 8, and the evaporation is controlled by the water vapor partial pressure until 100% relative humidity is achieved; (b) when the boiling temperature (determined by the air-water mixture pressure) is reached, water continues to evaporate according to Eq. 10. After the droplet evaporates due to either high temperature or low moisture partial pressure, the water vapor is transported away due to convection and diffusion as described in the water vapor species transport equation 4.

**CFD Model Results**

In DPM calculations, the droplet behavior and evaporation characteristics are treated globally as average properties in the injected parcels. Detailed local results, like pressure distribution or heat transfer coefficient along the surface and the temperature distribution inside the droplet, cannot be obtained. This lack of information obtained by CFD and thermodynamic calculations was the motivation to perform more detailed calculations using a single water droplet in an air stream in Approach 3. The result of droplet evaporation time and status (how much is evaporated) obtained from CFD model results will be used to compare with the result from Approach 3.

**Boundary Conditions**

The inlet condition of the domain is specified by a flow velocity. The outlet condition is set at the constant atmospheric pressure, and the sides of the domain are taken as periodic. Regarding the discrete phase, a mono-disperse spray composed of 4 streams is injected at the inlet of the duct. The base case parameters, according to typical droplet evaporation values, are shown in Table 1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Base Case Value (BC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet air temperature</td>
<td>310 K</td>
</tr>
<tr>
<td>Inlet air Velocity</td>
<td>1 m/s</td>
</tr>
<tr>
<td>Droplet Inlet Velocity</td>
<td>3 m/s</td>
</tr>
<tr>
<td>Droplet Re Number</td>
<td>2.63</td>
</tr>
<tr>
<td>Droplet diameter</td>
<td>20 µm</td>
</tr>
<tr>
<td>Droplet Temperature</td>
<td>300 K</td>
</tr>
<tr>
<td>Relative Humidity</td>
<td>60 %</td>
</tr>
</tbody>
</table>

Evaporation time (lifetime) of the droplets is the most favorable result sought. Figure 1(a) shows the variation of the droplet's diameter, velocity, and temperature. The lifetime of the droplets under base case conditions is 0.407 s. The variation in diameter also conforms with the $d^2$-law of droplet evaporation which can be expressed as

$$d_0^2 - d^2 = \lambda t \tag{11}$$

where $\lambda$ is the droplet evaporation constant obtained from the figure as $9.37 \times 10^{-10}$ (s/m²) for the base case.

Figure 1(b) shows the variation of the droplet velocity. The droplet quickly catches the main flow speed, due to its interaction with the air flow through drag, after a duration called the hydrodynamic response time which is approximately 0.004 s here. Similarly, Fig.1(c) shows the variation of the droplet temperature with a thermal response time of 0.0025 s.
Figure 1 Variation of the droplet characteristics (a) Normalized droplet diameter shown in d"-law (b) droplet velocity (c) droplet Temperature

II ZERO-DIMENSIONAL MODELS

1-D Lumped Capacitance Model

A water droplet evaporates due to the heat transfer between the surrounding medium and the droplet. It is hypothesized that, when the liquid water molecules evaporate on the surface of the liquid droplet, the latent heat is supplied by both the ambient air and the interior of the droplet with the fractions being correlated to the ratio of their corresponding equivalent thermal resistances, or Biot number. The energy associated with the phase change is the latent heat of vaporization of the liquid. Evaporation occurs when liquid molecules near the liquid surface experience collisions that increase their energy above that needed to overcome the surface binding energy. The energy required to sustain the evaporation must partially come from the internal energy of the liquid, which would then experience a reduction in temperature (The Cooling Effect). The latent energy lost by the liquid because of evaporation must be replenished by energy transfer to the liquid from its surroundings. Neglecting radiation effects, this transfer may be due to the convection of sensible energy from the gas or to heat addition by other means.

The existing built-in model in Ansys/Fluent models latent heat being absorbed only from inside the droplet and followed by transferring heat from the surrounding air to heat up the droplet, as shown in Eq. 6. Therefore, it is speculated that the previously observed situations—when the droplet temperature becomes very low and occasionally drops to below freezing temperature intermittently during evaporation process—were caused by the model formulated as Eq. 6. After the droplet temperature drops significantly, the subsequent heat transfer increases significantly to transport energy from the surrounding warmer air to quickly heat up the droplet. Although this behavior is transient and occurs intermittently and temporarily, it is not reasonable. This behavior should not be confused with the well-known droplet supercooling because the medium temperature (main stream), in our case, is well above the water freezing point. To investigate the proposed hypothesis, Eq. 6 will be modified to include a term which will allow energy to be transported to the liquid droplet surface from the surrounding air based on the Biot number. The modification is based on the following model development.

Consider an equivalent thermal circuit for heat transfer path between the hot gas and the droplet in a zero-dimensional lumped capacitance model as shown in Fig. 2a.

The Biot number, Bi, gives a simple index of the ratio of the thermal resistances inside and outside of the droplet. In the traditional definition of Biot number, conduction is treated as the dominant heat transfer mode; and no convection and associated internal flow activity are considered. This ratio also affects—although it does not necessarily determine—the corresponding fraction of heat that is transferred from outside versus from inside; thus, it affects the change of droplet temperature. The definition of Biot number is

\[
\text{Bi} = \frac{hL}{k_d} = \frac{R_{\text{cond}}}{R_{\text{conv}}} \tag{12}
\]

where \( h \) is the heat transfer coefficient of the gas and \( k_d \) is the thermal conductivity of the droplet. \( L \) is the characteristic length (taken as the droplet radius).

Estimates of the Biot number of two different droplet sizes at 20 \( \mu \)m and 1 mm are shown in Tables 2 and 3 respectively. The Ranz and Marshal correlations [6-7] are used to calculate Nu and, hence, the convective heat transfer coefficient.

![Energy Sink](image)

Figure 2a Thermal resistance circuit illustrates the hypothesis that the evaporation energy is sucked from both inside and outside of the liquid droplet.

<table>
<thead>
<tr>
<th>( U_{\text{slip}} ) (m/s)</th>
<th>Re</th>
<th>Nu</th>
<th>( h ) (W/m(^2)(\cdot)k)</th>
<th>Bi</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.01</td>
<td>2.06</td>
<td>2707.9</td>
<td>0.044</td>
</tr>
<tr>
<td>0.1</td>
<td>0.12</td>
<td>2.19</td>
<td>2876.6</td>
<td>0.047</td>
</tr>
<tr>
<td>1</td>
<td>1.23</td>
<td>2.59</td>
<td>3409.9</td>
<td>0.056</td>
</tr>
<tr>
<td>2</td>
<td>2.46</td>
<td>2.84</td>
<td>3732.9</td>
<td>0.061</td>
</tr>
</tbody>
</table>
Table 3 Lumped capacitance calculations for droplet with d=1 mm

<table>
<thead>
<tr>
<th>U_{slip} (m/s)</th>
<th>Re</th>
<th>Nu</th>
<th>h (W/m^2.K)</th>
<th>Bi</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>0.62</td>
<td>2.42</td>
<td>63.63</td>
<td>0.0519</td>
</tr>
<tr>
<td>0.1</td>
<td>6.16</td>
<td>3.33</td>
<td>87.48</td>
<td>0.0713</td>
</tr>
<tr>
<td>1</td>
<td>61.56</td>
<td>6.19</td>
<td>162.89</td>
<td>0.1328</td>
</tr>
<tr>
<td>2</td>
<td>123.12</td>
<td>7.93</td>
<td>208.58</td>
<td>0.1701</td>
</tr>
</tbody>
</table>

Although Biot number can help provide an idea of how thermal resistance ratio would affect heat flow distribution, the actual heat flow ratio (E_{\text{flow}}/E_{v}) is still undetermined until the temperature gradients are known on either side of the droplet-air interface. In principle, the lumped capacitance approach encounters some ambiguity because the temperatures inside a droplet are uniform and, hence, there is no temperature gradient inside the droplet. This ambiguity can be clarified by assuming the droplet temperature is at the center of the droplet, so the 1-D thermal circuit shown in Fig. 2 can be applied. The 1-D approach can also provide a quick estimate of Droplet Response Time and Evaporation Time.

**Droplet Hydrodynamic Response Time**

Both droplet drag and heat transfer depend on the slip velocity between the droplet and the air. The elapsed time (response time) of a particle to achieve the mean flow velocity and to reach the main flow temperature varies with the droplet size. The equation of motion for a spherical particle in the air is given by

\[ m \frac{dv}{dt} = \frac{1}{2} C_D \pi d^2 \rho_g \left( u - v \right) \left( u - v \right) \]  \hfill (13)

where \( u \) is the gas velocity and \( v \) is the droplet velocity.

Different hydrodynamic response times can be obtained by using different drag models. For example, by using the Stokes drag law, the hydrodynamic response time is obtained as

\[ \tau_h = \frac{\rho_d d^2}{18 \mu_g} \]  \hfill (14)

Following the Schiller and Neumann [22] drag model, the hydrodynamic response time can be obtained as

\[ \tau_h = \frac{\rho_d d^2}{18 \mu_g [1+0.15 \Re e^{0.687}]} \]  \hfill (15)

Similarly, the thermal response time (\( \tau_t \)) is defined as the elapsed time required for the droplet to achieve thermal equilibrium with the mean flow bulk temperature. It can be obtained from Eq. 6, assuming the temperature is uniform throughout the particle with negligible radiative effect as:

\[ \tau_t = \frac{\rho_d d^2 c_p}{6 \Nu K_g} \]  \hfill (16)

Estimate of different slip velocities and two different droplet sizes (20 \( \mu \text{m} \) and 1 mm) is shown in Table 4. The hydrodynamic response time ranges from 0.77 s to 0.95 s, while thermal response time is longer, around 3.06 s; whereas, the CFD calculations show much lower values (0.005 and 0.003, respectively)

**Droplet Evaporation Time** - Several models have been proposed for calculating droplet evaporation time in the open literature. Zheng et. al [23] modeled the droplet evaporation time as

\[ t = \frac{R_0 d^2}{8 \rho_d \nu (T_a - T_d)} \]  \hfill (17)

White and Meacock [24] proposed another droplet evaporation model as

\[ t = \frac{d^2}{8 \rho_d \nu D (T_{\text{sat}} / T_a)} \]  \hfill (18)

where \( \omega_0 = 0.02422 \) and \( \omega_1 = 0.02723 \) are the specific humidity (kg/kg dry air) at dry bulb and wet-bulb temperature, respectively. \( P_d = 3.567 \text{ kPa} \) is the droplet saturation pressure \( P_d = P_{\text{sat}} (T_d=300 \text{ k}) \), and \( D = 2.88 \text{E-05} \text{ m}^2/\text{s} \) is the diffusion coefficient. The estimated evaporation times using both models are shown in Table 5.

**Table 5 Evaporation time in the base case**

<table>
<thead>
<tr>
<th>Case</th>
<th>t (Zheng), s</th>
<th>t (White), s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base Case</td>
<td>0.00254</td>
<td>0.00052</td>
</tr>
</tbody>
</table>

A large difference is seen when the results from 1-D model are compared with that calculated by the CFD simulation in approach 1. It seems that the droplet evaporation time as calculated with Zheng’s model is twice longer than that calculated with White’s model.

**Modified droplet evaporation energy equation**

Considering the aforementioned effect of Bi, the droplet evaporation energy equation (Eq. 6) is therefore modified as:

\[ m_p c_p \frac{dt}{dt} = \pi d^2 h(T_\infty - T_d) + f(Bi) \frac{dp}{dt} h_{ig} \]  \hfill (19)

with \( f(Bi) \) being a function of Bi number and thermal response time. As Bi \( \rightarrow 0 \), the proposed function \( f \rightarrow 1 \), indicating that
all the latent heat comes from the droplet. On the other hand, when Bi → ∞, f→0 which means that convection term is dominant and energy is sucked from outside the droplet. The function (f) can be suggested to be in the exponential format as exp (- φBi). Where φ is a constant, related to the droplet evaporation rate, to be obtained from experiment.

This approach will allow less latent heat to be sucked from the droplet than Eq. (6) and will help avoid overcooling of the droplet. The remaining part of the work in Approach 3 will be dedicated to performing a detailed CFD calculation surrounding a single droplet without using the built-in droplet evaporation model and empirical equations.

(III) SINGLE DROPLET CFD SIMULATION WITHOUT USING BUILT-IN EVAPORATION MODEL

In this approach, the evaporation model of FLUENT is turned off, and evaporation is simulated by assigning a small amount of liquid evaporating from a very thin shell layer surrounding the droplet's surface. Then, the corresponding amount of latent heat required for evaporation is assigned as an energy sink in this thin evaporation layer. The evaporated water vapor on the droplet surface will be transported away from the surface. The local flow behavior and heat transfer will be calculated by the governing equations (Eq. 1-4), and no empirical correlations (Eqs. 7-10) will be used. The main objective is to calculate the heat flow distribution around the droplet surface and to determine the fraction of heat flow sucked from the droplet's interior versus from the surroundings. A transient CFD model is setup with a stationary droplet suspending near the inlet of a long 2D duct. The computational domain is constructed using Gambit, and the discretized control volume form of governing equations is solved using FLUENT. These calculations, compared to the built-in evaporation model, will give us the ability to do the following:

(a) Perform the evaporation process away from the suspected built-in evaporation model,
(b) Solve the flow field outside, as well as inside the droplet. (Unlike the DPM model which deals globally with the droplet parameters, the calculation procedure gives complete details of the flow field and the temperature inside the droplet.),
(c) Gradients inside and outside the droplet can be calculated and the relative amounts of heat (E_d and E_a) can be estimated.

To perform this task in the FLUENT environment, two features are used: Fixing of Solution Variables Technique and Source Terms.

Fixing the Solution Variables Method. This method gives the ability to deal with the droplet as a single phase liquid continuum fixed in the computational domain. It simply prevents solving the species transport equations in a specific part of the domain, which is the droplet volume in our case. In the present study, the mass fraction of liquid water is fixed as one to simulate a liquid droplet 100% water with the desired diameter. Accordingly, the species transport equation is not solved in the droplet volume to keep it always in the liquid phase although other transport equations (momentum and energy) are still solved to enable studying the flow and temperature fields inside the droplet. Without this treatment, the air will diffuse into the liquid droplet, and the liquid filaments can be seen to diffuse and be convected in the airstream. This treatment requires the creation of three different zones inside the computational domain: (a) the droplet zone with water liquid mass fraction of 1, (b) the shell zone around the droplet with mass source for water vapor and energy sink to simulate liquid evaporation, and (c) the outer domain represents the rest of the flow field. These three distinct cell zones are connected via non-conformal grid interfaces to allow the transport equations to be solved in the whole domain. These zones are schematically shown in Fig. 2b.

Source and Sink Terms- A positive mass source term (S_m and S_v in Eqs 1 and 4) is used to inject water vapor in the shell zone accompanied by the subtraction of a corresponding amount of energy via a negative energy source term (S_h in Eq. 3), as shown in Fig. 2b. This process forces the water vapor to be in the saturated state surrounding the liquid surface and is transported away by diffusion and convection. The heat flows will be naturally developed based on the property values and governing equations. It is important to mention that these added mass and energy sources are Volumetric Rate Sources, not cell sources. This means that the units must be (kg/m^3.s) and (W/m^3) respectively. This is performed by dividing the mass source by the shell volume and the estimated evaporation time calculated using the CFD calculations as shown in Fig. 1(a).

![Figure 2b Schematic shows the energy and vapor flow directions at the droplet surface (within the shell zone)](image)

**Technical Challenges**

1. During the CFD simulation, many technical challenges were encountered. Some of the major issues are described below. The water liquid was noticed to diffuse out of the droplet zone as a result of the diffusion term in the liquid water species transport equation. Of course, during the real droplet evaporation process only water vapor, not liquid water, diffuses outwardly from the droplet surface. Since the real physics does not involve this kind of liquid phase diffusion, it was necessary to stop this numerically induced error. To prevent the unreal diffusion of liquid water molecules, the liquid water species transport equation is forced not to be solved outside the droplet...
domain by fixing the mass fraction of water liquid to be always zero outside the liquid droplet.

2. The same problem happened to the water vapor outside the droplet zone; it started to diffuse into the droplet. This problem was similarly resolved by fixing the mass fraction of water vapor species to be always zero inside the droplet domain.

3. During the earlier stage of computation, the numerical iteration had always diverged without an apparent reason. Many efforts were spent on investigating the typical numerical procedures and issues that would lead to divergence without much success. Finally, it was discovered that the main reason of divergence was attributed to the mesh quality in the droplet-shell-domain interface. This interface problem was intricate and difficult to be identified; however, its effect is devastating. In one of the many different attempts to search for the answer to the divergence problem, the flow was solved in many steps with gradual complications, starting with only a solid droplet without a shell, and ending with the current problem formulation as shown in Fig. 4. It can be concluded that in any kind of problem which contains a non-conformal grid interface, it is necessary to implement very dense grid at the interface between two zones. This very dense grid reduces the irregularities on the matching interface zones and yields correct flux calculations through the interface zone.

4. Earlier results showed a great disparity in values of heat flux on two sides of the droplet interface. This disparity indicates that something is not correct in the computational process. After investigation, the built-in method of calculating the thermal conductivity and density in the commercial code was found to be the culprit. It gave the property values close to those of air and water vapor on both sides of the interface, rather than giving the property values of liquid water in the liquid domain. It was not clear how this would happen in a domain in which 100% of the material was assigned to be water, but this problem was resolved by adopting the mass weighted average method instead of the ideal gas method. When the ideal gas density calculation method was used in the whole domain (for pressure-based solvers), the droplet density was not correctly calculated. It appears that FLUENT used the properties of liquid and water vapor in the calculations for the liquid-only droplet. After investigation, the mass weighted average method was used to calculate density and thermal conductivity. It gave correct results for water density in the droplet domain after assigning the water vapor mass fraction as zero. The mass weighted average method along with the zero mass fraction of water vapor in the droplet zone removes any possibility of using water vapor properties in the calculations. It simply calculates the properties of the mixture as a simple mass fraction average of the pure species properties. For more details, see [20].

Mesh Generation

The grid consists of three separate cell zones: one for the droplet with diameter 20 µm, the second for a very thin shell layer around the droplet with a thickness of 0.2 µm, and the third represents the rest of the computational domain. The three separate cell zones are generated and meshed separately in Gambit, the preprocessor of the FLUENT package, and then are combined together in the solver. GAMBIT generates structured (mapped), unstructured (paved), and hybrid meshes. The mesh used for the model is mainly unstructured except inside the thin shell layer wrapping around the droplet surface and near the interfaces between the droplet, the shell, and the rest of the domain. At these interfaces, the mesh takes the form of structured grid called boundary layer (B.L.) mesh which gives a good resolution at these boundaries with a large gradient in the solution variables. Great care must be taken in generating the mesh at these interfaces to prevent any possible mismatching of the non-conformal grid interface. This could be a main source of divergence and errors during calculation. To avoid these problems, the mesh is designed to be greatly clustered around the interfaces to give a better geometrical resolution, as shown in Fig. 4a. An amplified view of Fig. 4a shows the details of the interfaces in Fig. 4b.

As mentioned earlier, great care must be taken in generating the mesh at interfaces which require the clustering of the mesh at these places. Accordingly, the mesh size was successively increased to achieve that purpose and produced a well-converged solution. Taking into account that the flow is laminar and two dimensional, the final mesh size of 139,531 cells was considered sufficient to perform the calculations of the base case. A grid sensitivity study was performed The mesh sensitivity study was done using a mesh adaption technique. Basically, the solution is calculated first with the primary mesh (139,531 cells), and all the solution variables are recorded. Then the mesh is adapted (refined) in two consecutive steps, namely, boundary adaption around the interfaces followed by volume adaption to achieve a smooth volume transition between cells. After the mesh adaption procedure is done, the solution is recalculated on the refined mesh and solution variables values are compared to the primary mesh before any adaption. The whole adaption and comparison process is repeated three times increasing the mesh size to 165K, 201K, and 341K cells, respectively. This adaption yields a final mesh size which is 2.5 times the original one. The results of the mesh sensitivity study are shown in Table 6 below. All solution variables are compared but only mass fraction of water vapor and static temperature at exit of the domain are shown here before and after the third adaption. It is clear from the third adaption (refinement) that increasing the mesh size 2.5 times only changes the solution variables by less than 3 % (2.8 %). It is clear that the solution is almost mesh independent.

<table>
<thead>
<tr>
<th>Table 6 Mesh sensitivity study results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exit vapor mass fraction (-)</td>
</tr>
<tr>
<td>Exit Static Temperature (K)</td>
</tr>
</tbody>
</table>
step sizes are used to calculate the solution, and the solution results are compared with the original time step size results. Results of the time step size analysis are shown in Table 8. It is clear that the solution is time step size independent because increasing or decreasing the time step size an order of magnitude has a negligible effect on the solution variables.

Table 7 Base case parameters.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Base Case Value (BC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air temperature</td>
<td>310 K</td>
</tr>
<tr>
<td>Inlet Air Velocity</td>
<td>1 m/s</td>
</tr>
<tr>
<td>Inlet RH</td>
<td>0</td>
</tr>
<tr>
<td>Droplet Re</td>
<td>2.63</td>
</tr>
<tr>
<td>Droplet diameter</td>
<td>20 µm</td>
</tr>
<tr>
<td>Droplet temperature</td>
<td>300 K</td>
</tr>
<tr>
<td>Shell Thickness</td>
<td>0.2 µm</td>
</tr>
<tr>
<td>Water Vapor Mass Source</td>
<td>1 % of the droplet Mass</td>
</tr>
</tbody>
</table>

Table 8 Time step size (s) sensitivity study results (change from the base case of 2.713 E-04 s)

<table>
<thead>
<tr>
<th>Change in exit vapor mass fraction</th>
<th>2.713 E-05</th>
<th>2.713 E-04</th>
<th>2.713 E-03</th>
</tr>
</thead>
<tbody>
<tr>
<td>Change in exit static temperature</td>
<td>0.00032</td>
<td>0 %</td>
<td>0.00032 %</td>
</tr>
</tbody>
</table>

Static temperature results

The results of static temperature in the base case are shown in Fig. 5. Figure 5(a) displays the temperature in the whole domain and Fig. 5(b) shows an enlarged view of the temperature field near and inside the droplet. The isotherms in Fig. 5(b) take almost concentric circles in the vicinity around the droplet. This isotherm pattern is expected due to the dominance of diffusion effects in this case because of the small Reynolds number of 2.6. This means that the forced convection effects are negligible. Therefore, the heat transfer is due mainly to the natural convection and the heat diffusion. The effect of natural convection can be discerned by the slightly asymmetric isotherm pattern in Fig. 5(a) with a bit more rising isotherm in the upper domain downstream of the droplet.

Figure 5(b) shows the temperature distribution inside the droplet is uniform due to its low thermal resistance. This agrees with the Biot number results obtained in the second approach of the paper using the lumped capacitance method.

Finally, the droplet temperature reaches the steady-state temperature about 304 K, which is 4 K higher than its initial temperature. This means that the droplet passed the transient heat-up period by absorbing heat from the surrounding air.

Velocity results

Figure 6(a) shows the velocity field inside the droplet. The internal free-convection (flow) is described by the Rayleigh number, which compares buoyancy forces (causing
convection) to diffusive and viscous forces (working against it). For our situation, the Rayleigh number can be defined as follows [25]:

$$Ra = g \frac{\Delta \rho}{\rho} \frac{d^3}{\nu D}$$

(20)

where $g$ is the gravitational acceleration, $\Delta \rho / \rho$ the reduced density difference, $\nu$ the kinematic viscosity and $D$ the diffusion coefficient. If $\Delta \rho / \rho$ is considered to be 1% with $\nu = 10^{-6}$ m$^2$/s and $D = 10^{-5}$ m$^2$/s, $Ra$ is about 9.81 for 1 mm droplet and $Ra=0.785$ for 20 µm diameter droplets. Small values of $Ra$ shows that the internal free-convection (flow) is negligible in case of small droplets, however in large droplets, the free-convection effect becomes noticeable.

Again, thanks to this detailed calculation procedure, the flow field detail inside the droplet is available. There are many induced vortices known in literature as Marangoni Instability, which results from the surface tension gradient. This gradient is caused by the non-uniform temperature distribution at the surface which occurs due to a high evaporation rate in this small size droplet. This surface tension gradient produces a force in which surface fluid is pulled toward regions of higher surface tension. The viscous force then transports momentum into the interior of the droplet and a convective flow results throughout the droplet. This surface-tension-driven instability flow was described by Cloot and Lebon (1990) and was experimentally visualized by Hegseth et al. (1996). As shown in Fig. 6(b), regarding the flow field around and behind the droplet, it is stable with minimum laminar wake structure due to the very small $Re$ number. The boundary layer can be also clearly seen over the droplet surface Fig. 6(b).

Figure 6 Velocity field (m/s) (a) Inside the droplet (b) behind the droplet

Water vapor distribution

The result of water vapor mass fraction (concentration) distribution in the base case is shown in Fig. 7. Figure 7(a) displays the water vapor mass fraction in the whole domain. Inlet water vapor mass fraction value is set zero (dry free stream) to allow a clear demonstration of the evaporation process. The pattern of water vapor concentration contour lines is similar to the isotherm pattern shown in Fig. 5, so the underlying physics is similar: the mass diffusion process is dominant near the droplet with slight enhancement due to natural convection. Although the effect of gravity enters the governing equations only via the momentum equation with the Boussinesq approximation, the temperature field affects the water vapor concentration and accordingly its transport indirectly.

Figure 5 Static temperature contour distribution in (a) the whole domain (b) enlarged view near the droplet
The respective heat flux distributions through the droplet surface and the shell outer surface are plotted in Fig. 9 versus the circumferential angle after 3 time steps ($t = 0.000814 \text{ s}$). As the temperature of the droplet is lower than the freestream temperature, the temperature gradient (as shown in Fig. 5) is negative in the direction from the flow to the droplet. This means that the heat flux (which is of the opposite sign) is positive from the flow to the droplet. Consequently, the heat is entering the droplet, resulting in an increase of the droplet’s temperature until steady state equilibrium is reached. This temperature change is clear in Fig. 1(c), where the droplet temperature increases first (heat-up period) and then stays constant during evaporation. Also, as the temperature of the droplet increases, the temperature gradient decreases causing the heat flux entering the droplet to reduce until the heat flux becomes zero when steady-state equilibrium is reached. This interprets the results depicted in Fig. 1(c) showing the steady-state equilibrium temperature of the evaporating droplet. Moreover, Fig. 10 clearly shows that the heat flux entering the droplet is greatly reduced after 1000 time steps ($t = 0.0271 \text{ s}$). Figure 11 shows the temperature vs. time diagram for a point at the droplet center. It is clear that the temperature, which was initially $300 \text{ K}$, increases with time until it reaches the steady-state equilibrium temperature as shown previously in Fig. 1(c). The droplet temperature is always increasing and never decreases. This above description of physics illustrates a different process from the built-in evaporation model centered at Eq. 6, which shows the potential for reducing the droplet temperature if the latent heat term is larger than the heat convection term.
Some extra notes can be mentioned about Figs. (9 – 11). First, the heat flux plotted in Fig. 9 seems to reveal that more energy is entering the droplet zone than the energy entering the shell, which is not the correct interpretation. The true picture can be seen as the heat fluxes crossing over the shell interface is adjusted for its approximately 4% larger surface area than the droplet interface surface area. This Area-Adjusted Heat Flux (AAHF) is shown as the dotted blue curve, which almost coincides with the curve representing the heat flux entering the droplet excluding the local heat flux maxima. Second, the highest heat flux occurs near 30° from the leading edge. The second highest heat flux occurs at the leading edge and the third heat flux peak occurs at around 90° from the leading edge. These local maxima all occur during the earlier transient period. When the time step reaches 0.0271, those secondary local maxima are smoothed out and the heat flux has significantly decreased to about an order magnitude smaller. The maximum heat flux occurs at the familiar location -- at the stagnation point as shown in Fig. 10. The temperature at the droplet’s center, Fig. 11, seems to follow a continuously increasing trend, even at 0.016 second. A coarse extrapolation gives a thermal response time of approximately 0.02 seconds to reach 302K. These 0.02 seconds of thermal response time is about an order of magnitude longer than 0.0025 seconds obtained from Eq. (11) in Fig. 1(c). This discrepancy is caused by the employment of a constant droplet size, rather than using a diminishing droplet size in the current DFD model.

To show the effect of Reynolds number on the calculations, a larger droplet size (1 mm) is used with the same inlet air velocity of 1 m/s to yield a Reynolds number of Re = 61.6. Higher inlet air temperature of 400 K is used in this case to drive a significant temperature gradient through the droplet. The rest of the parameters are kept as in the base case of 20 μm droplets. As the Reynolds number increases, it can be clearly seen in Fig. 12 that the convection effect becomes dominant. Moreover, as the droplet size increases, the temperature distribution inside the droplet becomes more uniform, and Marangoni instability and natural convection start to occur inside the droplet, as shown in Fig. 13. The bigger the droplet size is, the more the conduction resistance is inside the droplet. This leads to an increased temperature gradient inside the droplet (around 5 degrees difference in temperature inside this droplet of 1 mm diameter).

From the calculations of Biot number (0.1328) for this 1mm droplet (shown in Table 3), a large temperature gradient is expected inside the droplet; thus, a lower amount of heat is sucked from the droplet due to its higher thermal resistance. However, unexpectedly, the results obtained earlier in Figs. 5, 9-13 show a different situation. All these figures show that the heat is transferred from the main flow to the droplet for different conditions of droplet size, and main stream temperatures and the droplet temperature never reduces.

**Figure 11 Temperature vs. time diagram for a point at the droplet center (20 μm droplet)**

**Figure 12 Effect of increased Reynolds number: static temperature contour distribution in (a) the whole domain (b) near the droplet (1 mm diameter droplet, Re =61.6)**

**Figure 13 Static temperature contour inside the droplet (1 mm diameter and droplet Re = 61.6).**

The question now is how to interpret the droplet temperature reduction observed in using the built-in evaporation model in the commercial code. The plausible answer is that when the droplet evaporation rate is extremely high, the amount of energy sucked at the droplet surface is so
high to the degree that part of the evaporation energy is sucked from the droplet, resulting in a momentary reduction of droplet temperature. To showcase this high evaporation rate scenario, a number of cases have been conducted with high evaporation rates by implementing high mass sources and negative energy sources at the droplet surface. Unfortunately, none of them gave a converged solution. Divergence was always detected at the beginning of the calculation as a result of the increased fluxes through the interfaces. That unstable behavior prevented the authors from showcasing that the droplet temperature can ever reduce.

CONCLUSIONS

This study is motivated by the observation of the droplet temperature’s temporarily dropping too low during evaporation process when a built-in evaporation model is used in a commercial CFD code. Three approaches have been made: (a) using the build-in evaporation model with empirical equations, (b) using a zero-dimensional analysis, and (3) using a commercial CFD to directly calculate the local heat transfer around a droplet without using the built-in empirical equations. (Note: This is not the direct numerical analysis or DNS.) The objective of this work is to understand the process and identify the problem of the built-in evaporation models available in most commercial codes.

The result of the zero-dimensional analysis indicates that the droplet temperature always increases. The direct CFD result also draws the same conclusion that the droplet temperature never drops during the evaporation process. A modification of the droplet temperature equation is proposed with a factor added to account for the effect of Biot number, which would reduce the latent heat to be sucked from the liquid droplet. The direct CFD method adequately captures the flow structure and Marangoni motion inside the droplet and provides information of heat flux surrounding the droplet.

ACKNOWLEDGEMENT

The authors want to thank Louisiana Governor’s Energy Initiative to support this project via the Louisiana Board of Regents and the Clean Power and Research Energy Consortium (CPERC).

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