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A Numerical Study on Droplet Evaporation using Mass and Heat Transfer Approach

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Abstract

Liquid fuel is injected into many combustion devices like engines, boilers, and gas turbines where it evaporates, mixes with air, and finally burns. The combustion process influences by evaporation and corresponding air-fuel mixing. Hence, the evaporation study of the fuel droplets is important in different thermodynamic conditions. In the present paper, fuel droplet evaporation has been numerically studied by two different approaches i.e., mass transfer and heat transfer. Multiple case studies have been conducted by varying the droplet surface temperature, its initial diameter, and the temperature of ambiance to understand the influence of each parameter on the evaporation process by the two different concepts. Transfer numbers (B), evaporation constants (K), and droplet lifetime are obtained through both heat and mass transfer models. These observations are highly helpful to understand the droplet evaporation process and comparing the two different approaches to droplet evaporation modeling.

Keywords: *Droplet Evaporation, Heat Transfer Approach, Mass Transfer Approach*

1.0 Introduction

As a part of analyzing engineering problems that involve spray combustion like liquid-fueled rockets, gas turbines, diesel engines, oil-fired boilers, process heaters, and furnaces, the knowledge of evaporation characteristics of a single droplet is highly essential. This gives a better understanding of the prediction of spray behavior[1-2]. When a liquid droplet is suddenly placed into a high-temperature ambiance, the temperature of the droplet also increases rapidly. A number of models have been developed over decades for the accurate estimation of the evaporation rate of an individual droplet. Modeling of a spherical liquid droplet that surrounded by gases to study the evaporation characteristics was first considered by Maxwell[3]. The evaporation process was described with the assumption that the rate of evaporation can be completely determined by the rate of diffusion from droplet to ambient gas. At the condition where the concentration of vapor around the droplet surface is equal to the concentration of vapor at the liquid-vapor equilibrium phase, a mathematical correlation has been deduced to calculate the change in droplet diameter with time[4-9].

Another model for multi-component spherical droplet evaporation had been developed by Tonini and Cossali[10] which was based on Stefan-Maxwell equations. The results were compared with Fick's law predictions under steady-state isothermal conditions for a wide range of gases, ambient temperatures, and droplet compositions. But the results were not well agreed and the rate of evaporation was underestimated particularly at higher temperatures[11]. Fuchs suggested that a small thickness of kinetic layers that surrounds the spherical droplet could describe the evaporation rate and can be calculated using the Hertz-Knudsen equation. This model neglects the mass diffusion process and exclusively depends only on kinetic theory[12]. Hence, an optimal model for the estimation of the evaporation rate should contain both mass and heat

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transfer descriptions[13]. For this, it is needed to know the individual effect of both heat and mass transfer processes and compare the results estimated by using the existing models.

2.0 Droplet Evaporation Models

2.1 Evaporation Model Based on Mass Transfer Approach

Evaporation of an individual droplet which is held in a quiescent ambience could be analyzed based on the mass transfer approach. Let, for an evaporating droplet, r_s is the droplet radius at the liquid-vapor interface. The mass fraction of the fuel vapor at the droplet surface is taken $Y_{As,}$ whereas the mass fraction at a large distance from the droplet surface ($r \to \infty$) is denoted by $Y_{A\alpha}$. During evaporation of the liquid droplet, the vapor from its surface will diffuse into the surrounding gas, which causes the loss of mass and ultimately results in a decrement of droplet radius along with the time.

This evaporation process can be numerically studied by determining the mass flow rate of the vapor from the droplet at any given time using conservation laws. To reduce the number of unknowns and equations, some assumptions are needed to be considered for a 1-D cartesian problem which are stated below.

- The entire evaporation process is considered to be quasi-steady, which helps for eliminate PDE.
- The droplet temperature is assumed to be uniform and is fixed at some value lower than the Boiling Point (BP) of liquid.
- The mass fraction of vapor at the droplet surface is determined only at the temperature of liquid-vapor equilibrium.
- All thermos-physical properties are considered to be constant.

With all the above assumptions, the following numerical equations have been obtained when law of conservation of mass is applied. The evaporation rate is calculated by,

$$m^{\cdot} = 4\pi r_s \rho D_{AB} \ln\left[\frac{\left(1-Y_{A,\infty}\right)}{\left(1-Y_{A,s}\right)}\right] \qquad (1)$$

Where, ρ = density of surrounding gas; and D_{AB} is binary diffusivity.

For better understanding how the mass fractions at $Y_{A,s}$ and $Y_{A,\infty}$ affect the evaporation rate, the logarithmic part of Equation (1) will be used to calculate dimensionless transfer no, B_Y.

$$B_Y = \frac{\left(Y_{A,s} - Y_{A,\infty}\right)}{\left(1-Y_{A,s}\right)} \qquad (2)$$

Hence,

$$m^{\cdot} = 4\pi r_s \rho D_{AB} \ln(1+B_Y) \qquad (3)$$

Similarly, by droplet mass conservation, the evaporation constant K is calculated.

$$K = \frac{8\rho D_{AB}}{\rho_l} \ln(1+B_Y) \qquad (4)$$

Where, ρ_l = density of liquid drop. The time for complete evaporation (or droplet lifetime) with respect to diameter can be given by the below equation.

$$t_d = \frac{D_0^2}{K} \qquad (5)$$

2.2 Evaporation Model based on Heat Transfer Approach

The rate of evaporation for the liquid droplet, which is surrounded by high-temperature gas, is generally controlled by the heat transfer mechanism. This can also be modeled with the help of the same spherically symmetric coordinate system with a few assumptions which are stated below.

- The evaporation process takes place in a quiescent, infinite medium and is quasi-steady for the sake of eliminating PDE.
- The droplet is of a single component and with zero solubility of gases.
- The temperature of the droplet is uniform and is assumed to be the same as its boiling point to avoid the need of solving fuel vapor transport equations.
- Lewis's member is assumed to be unity ($\alpha = D$) in binary diffusion which permits to apply simple shvab-zeldovich energy equation.
- All thermos-physical properties are assumed to be constant.

By applying the relevant boundary conditions and integrating the energy conservation equation, the evaporation rate can be given by below equation,

$$m^{\cdot} = \frac{4\pi k_g r_s}{c_{pg}} \ln\left[\frac{c_{pg}(T_\infty - T_{boil})}{h_{fg}} + 1\right] \quad (7)$$

The term in brackets of Equation (7) could be known as Spalding number or transfer number and could be denoted with B_q.

$$Bq = \frac{c_{pg}(T_\infty - T_{boil})}{h_{fg}}$$

$$m^{\cdot} = \frac{4\pi k_g r_s}{c_{pg}} \ln\left[\frac{c_{pg}(T_\infty - T_{boil})}{h_{fg}} + 1\right]$$

$$m^{\cdot} = \frac{4\pi k_g r_s}{c_{pg}} \ln\left(B_q + 1\right) \quad (8)$$

Evaporation constant is

$$K = \frac{8k_g}{\rho_l c_{pg}} \ln\left(B_q + 1\right) \quad (9)$$

Droplet life time can be given by the below equation,

$$t_d = D_0^2 / K \quad (10)$$

By following the approach of Law and William, c_{pg} and k_g have been derived by the below equations.

$$c_{pg} = c_{pF}(\bar{T}) \quad (11)$$

$$k_g = 0.4k_F(\bar{T}) + 0.6k_\infty(\bar{T}) \quad (12)$$

where, $\bar{T} = (T_{boil} + T_\infty)/2$

3.0 Methodology

To analyze the evaporation characteristics through mass and heat transfer approach, n-hexane has been selected as a reference fuel. Number of numerical cases have been analyzed by varying droplet initial diameter, ambient temperature and droplet surface temperature. This will help to know the effect of each parameter on the rate

Table 1. Properties of various fuels

Fuel	Density (kg/m^3)	Boiling point (K)	Latent heat of evaporation, h_{fg} (kJ/kg)	Mol. wt (g/mol)
n-Hexane(C_6H_{14})	659	342.15	335	86.18
n-Octane(C_8H_{18})	703	398.85	300	114.26
n-Decane ($C_{10}H_{22}$)	730	447.25	277	142.29

Table 2. Condition for droplet evaporation study by Mass transfer approach

Case No	Purpose of the study	Fuel	T_{amb} (K)	*T_{surf} (K)	Droplet initial diameter (μ m)
1	Effect of droplet Surface temperature	C_6H_{14}	600	-	100
2	Effect of droplet initial diameter	C_6H_{14}	600	T_b -0.001	-
3	Effect of ambient temperature	C_6H_{14}	-	T_b -0.001	100
4	Effect of fuel	-	600	T_b -0.001	100

* It is noted that, in the mass transfer approach, it is assumed that the droplet surface temperature is below the boiling point of the liquid. The surface temperature effect is studied in case 1. In other cases, the surface temperature is kept very close to the boiling point (T_b-0.001).

Table 3. Condition for droplet evaporation study by Heat transfer approach

Case No	Variable Parameter	Fuel	T_{amb} (K)	T_{surf} (K)	Droplet initial diameter (μ m)
1	Effect of droplet initial diameter	C_6H_{14}	600	T_b	-
2	Effect of ambient temperature	C_6H_{14}	-	T_b	100
3	Effect of fuel	-	600	T_b	100

of evaporation through both modeling processes. Later, the results obtained using n-hexane droplets have been compared with other fuels (n-Octane and n-Decane) to understand the effect of fuel properties on droplet evaporation. Table 1 shows the properties of the fuels. Table 2 and Table 3 show the different conditions considered for droplet evaporation study by the two approaches.

4.0 Results and Discussions

The variations of droplet diameter with respect to time is calculated by the mass and heat transfer approach as explained before. All the equations are coded through MATLAB for the ease of calculations. The results are discussed below.

4.1 Droplet Evaporation by Mass Transfer Approach

4.1.1 Effect of Droplet Surface Temperature

To study the effect of droplet surface temperature on the evaporation process, five different temperatures including one very close to its boiling temperature (T_b-0.001) have been selected. For the analytical calculation by mass transfer approach, it is not feasible to consider surface temperature (T_s) equal to boiling temperature (T_b). It is because, considering $T_s = T_b$, leads to mass fraction of liquid at the droplet surface equal to 1 and finally Transfer number, By = infinity. Hence it is considered as $T_s = T_b$-0.001 which is approximately equal to the boiling temperature. By keeping the ambiance temperature (600K) and droplet initial diameter (100µm) constant, the results are represented in Figure 1. It can be observed that, with the decrease of droplet surface temperature from its boiling point, the evaporation rate is increased. A decrease in surface temperature reduces the fuel mass fraction at the droplet surface which leads to a decrease in the Transfer number, which finally decreases the evaporation constant. As a result, the evaporation process slows down at the lower surface temperature of the droplet.

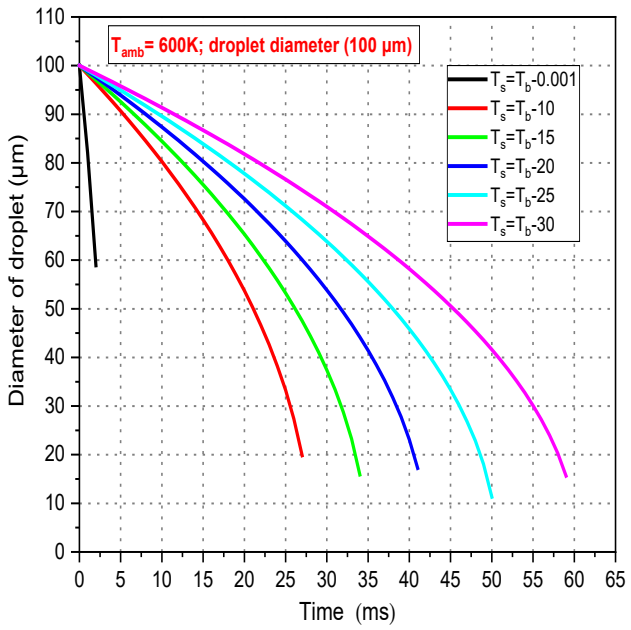

Figure 1. Variation of droplet diameter with time at different surface temperatures by mass transfer approach.

4.1.2 Effect of Ambient Temperature

To study the effect of ambient temperature on the evaporation process, the droplet surface temperature and droplet diameter (100µm) are kept constant and ambience temperature are varied. Left of Figure represents the results of where droplet surface temperature is considered as very close to its boiling temperature ($T_s = T_b$-0.001°C). It can be observed that changing the ambiance will not affect the droplet lifetime to a great extent in the mass transfer approach. But the effect of ambient temperature can be observed when the surface temperature is below its

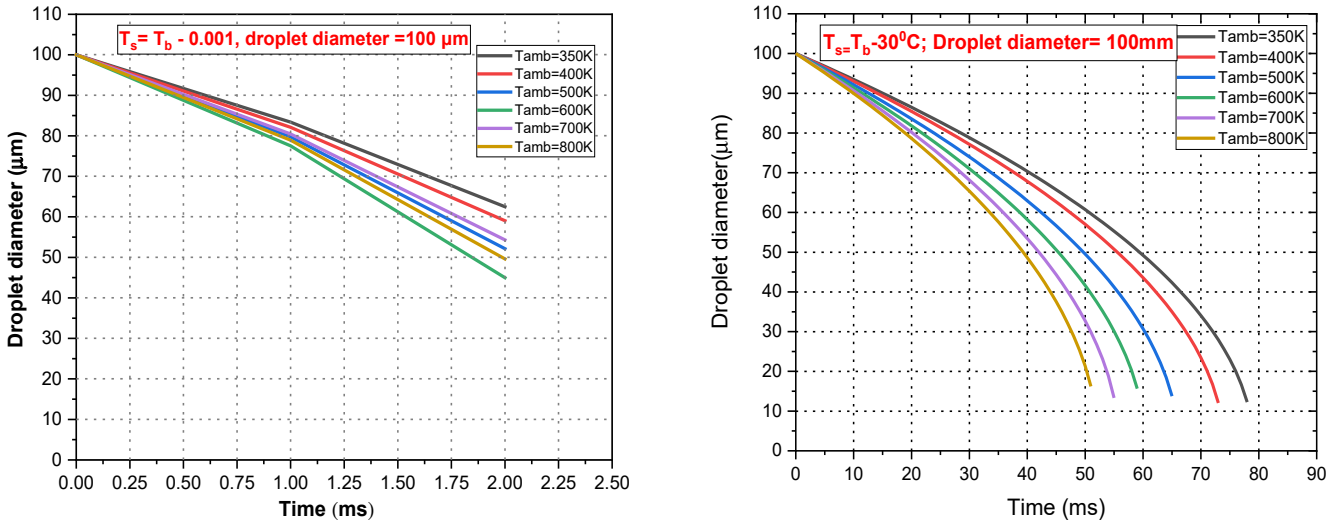

Figure 2. Variation of droplet diameter with time at different ambient temperatures by mass transfer approach at Ts = Tb-0.0010C (Left) and Ts = Tb-300C (Right).

boiling temperature as shown in Right of Figure 2 where droplet surface temperature is considered 30 degree below to its boiling temperature ($T_s = T_b - 30^0C$).

4.1.3 *Effect of Droplet Diameter*

The initial droplet diameter also affects the droplet evaporation time as the rate of diffusion is inversely proportional to the size of droplet. Figure 3 represents the variation in droplet diameter with time for different droplet initial diameters at constant ambient temperature T_{amb} = 600 K and surface temperature $T_s = T_b$-0.001°C. The figure shows that at same conditions, the droplet life time is higher for the droplets with bigger initial diameter (Figure 3).

4.1.4 *Effect of Fuel*

As every fuel is differed in their physical and chemical properties, the effect of fuel on the evaporation process

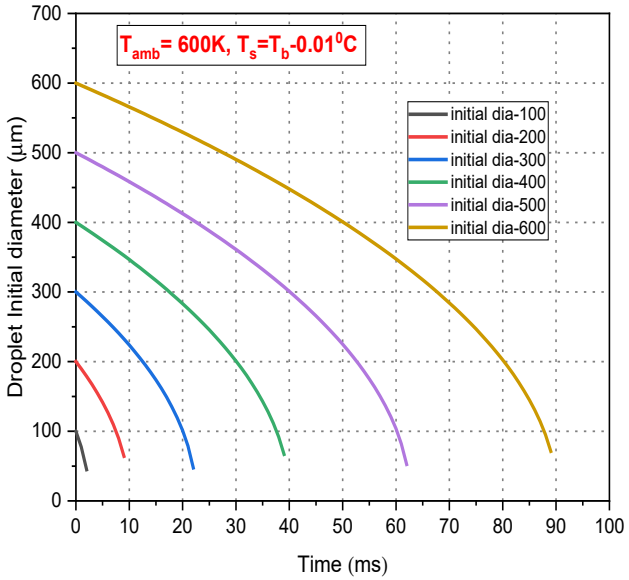

Figure 3. Variation of droplet diameter with time for different initial diameters by mass transfer approach.

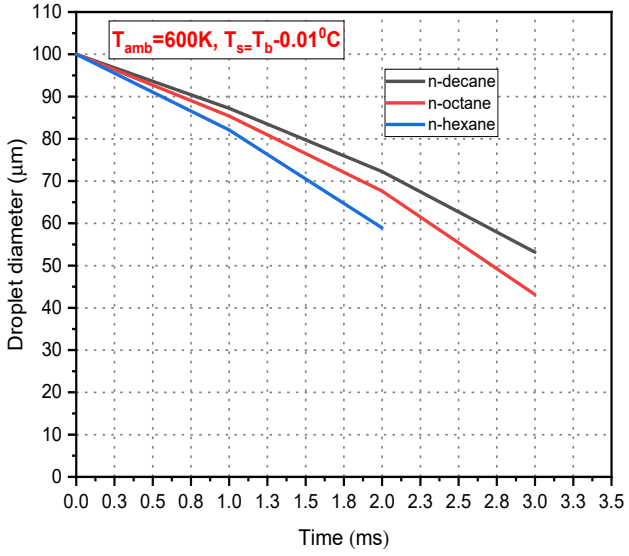

Figure 4. Variation of droplet diameter with time at different surface temperatures by mass transfer approach.

should be studied. For that, three different fuels, n-decane, n-octane and n–hexane are considered. The initial diameter and ambient temperatures are considered same and surface temperature is taken very close to its boiling temperature (T_b-0.001). From Figure 4 it can be noticed that, as the density of the fuel decreases, mass transfer rate increases which leads to faster evaporation rates.

4.2 Droplet Evaporation by Heat Transfer Approach

4.2.1 Effect of Ambient Temperature

The droplet evaporation process is highly affected by heat transfer process, particularly at higher temperatures. As per the assumptions in the heat transfer approach, the surface temperature of the droplet should be considered at its boiling temperature. The diameter of the droplet (100μm) is also kept constant for all cases. The variation of droplet diameters at different ambient temperatures are calculated and shown in Figure 5. It can be observed

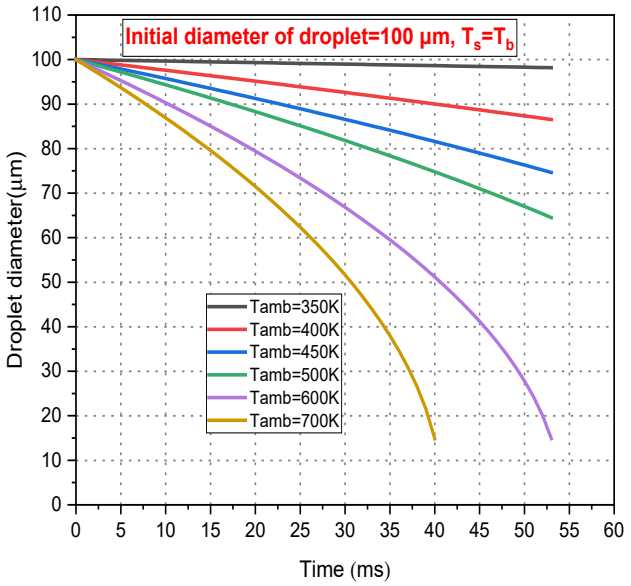

Figure 5. Variation of droplet diameter with time at different ambient temperatures by heat transfer approach.

that the droplet evaporation rate is higher for the high ambient temperatures.

4.2.2 Effect of Droplet Initial Diameter

Varying the initial droplet diameter cause a great impact on droplet life-time. By keeping the ambient temperature

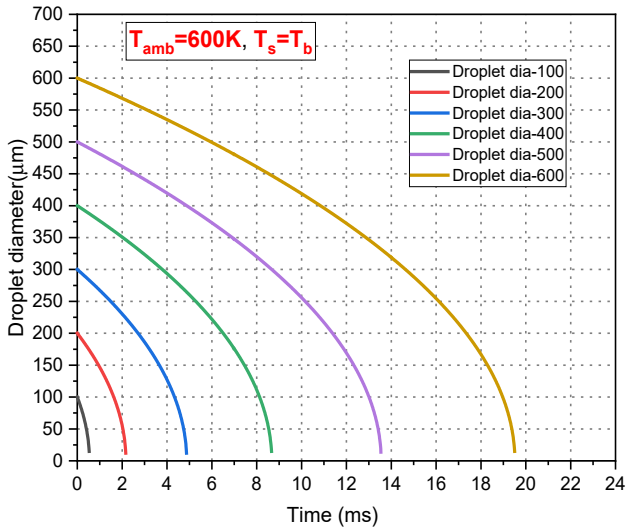

Figure 6. Variation of droplet diameter with time for different initial diameters by heat transfer approach.

and surface temperature same for all cases, the evaporation rate is calculated for different initial diameter and the results are shown in Figure 6. It is seen that like mass transfer approach, heat transfer mechanism also shows similar trends i.e., greater the initial diameter, greater the droplet life-time.

4.2.3 Effect of Fuel

Same fuels that have been taken before in mass transfer analysis, have been considered in heat transfer approach.

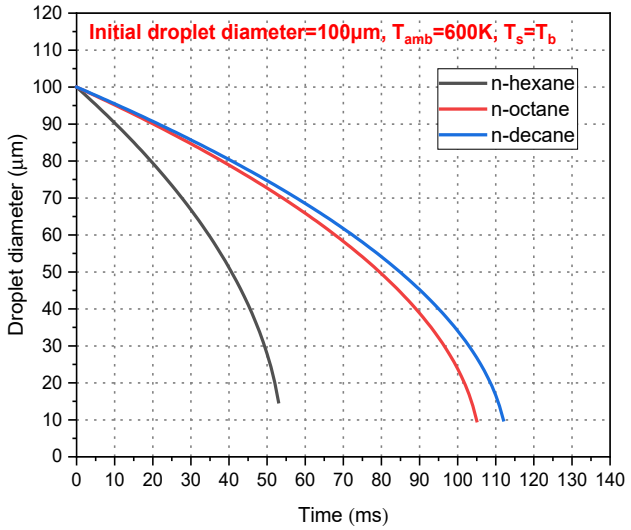

Figure 7. Variation of droplet diameter with time for different fuels by heat transfer approach.

The ambient temperatures and droplet initial diameter are also maintained as before i.e., 600 K and 100 microns. From the Figure 7, it can be observed that the droplet life-time is less for the low-density droplets using heat transfer approach which is same as mass transfer approach.

5.0 Comparison between Heat and Mass Transfer Approaches

To understand the difference between the two approaches of droplet evaporation, a comparison study has been conducted at same conditions. N-hexane is considered as reference fuel and the initial droplet diameter is taken as 100µm. Surface temperature is to be considered as its boiling temperature for heat transfer approach and very close to boiling temperature (T_b-0.001) for mass transfer approach. Three different ambient temperatures (350K, 500K and 600K) are considered. The results are shown in Figure 8. From the figure, it can be observed that, although the droplet surface temperature is almost equal in both heat and mass transfer cases, an increment

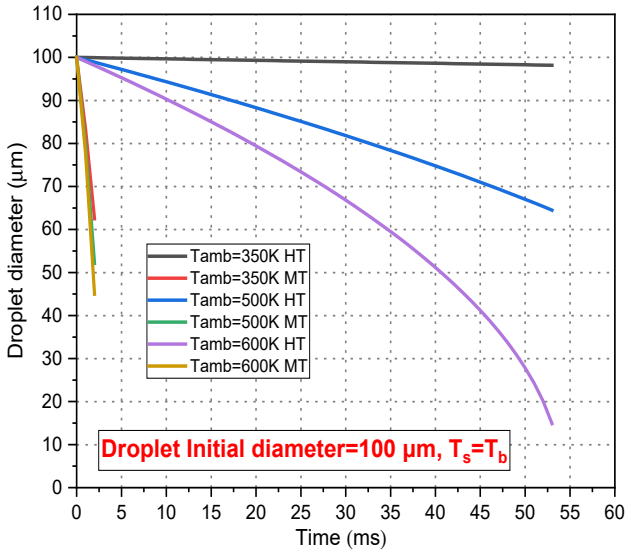

Figure 8. Variation of droplet diameter with time.

in ambient temperature showed more effect on the heat transfer approach but negligible effect on the mass transfer approach. This comparison helps to understand how the evaporation process is being affected at different ambient temperatures by both modeling processes.

6.0 Conclusions

As the mass and heat transfers affect the evaporation process of a droplets, numerical analysis has been done for each approaches and the results are analyzed for each case. From analyzing the results, the following conclusions have been drawn.

- For mass transfer approach, surface temperature plays an important role. Higher is the surface temperature, higher is the droplet evaporation rate.
- For mass transfer approach, if the surface temperature is close to boiling temperature, surround gas temperature does not effect the evaporation rate. However, evaporation rate is influenced by ambient temperature if the surface temperature is much below the boiling temperature.
- In heat transfer approach, ambient temperature plays an important role in droplet evaporation. Higher ambient temperatures increase the rate of evaporation.
- For both the approaches, smaller droplet diameter evaporates faster.
- For heat or mass transfer approaches, decrease in fuel density increase the rate of evaporation.

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