

Effect of Initial Temperature and Diameter of Ethanol Droplet on Evaporation Dynamics in Convective Air Medium

Numan Siddique Mazumder^{1*}, Pradip Lingfa², Asis Giri³

Abstract

Ethanol is a suitable biofuel as it has fewer toxic emissions and higher-octane numbers. For spray combustion applications, the gas phase motion must be considered while numerically investigating the fundamental aspects of droplet evaporation and combustion processes. Hence, we have numerically simulated the evaporation dynamics of an isolated spherically shaped ethanol droplet under a forced convective air environment in the absence of gravity. The momentum transfer between two phases is captured by incorporating the Navier-Stokes equation into the spherical polar coordinate system. The governing equations of species, motion, and heat transfer are solved with the aid of the finite difference method. The variable blowing effect (Stefan flow), unsteady droplet heating, and non-unitary Lewis number are considered in the mathematical formulation. The Reynolds number is considered 100 at an ambient temperature of 600 K. The present work is validated by comparing the d^2 -curve of an ethanol droplet with the literature. A parametric study was performed to examine the effects of droplet initial diameter and temperature. The diameter is considered in the range of 0.2 mm to 1.0 mm, while the internal temperature is varied from 290 K to 325 K. The results reveal that droplets with a smaller diameter evaporate early, and the heat-up period is less compared to the bigger droplet. Moreover, a droplet with a higher internal temperature has a relatively shorter life span compared to one with a lower internal temperature. Also, the streamline, isotherm, and species concentration contour plots of the evaporating droplet have been shown.

Keywords: Biofuels, evaporation, Navier-Stokes equation, force-convection, diameter, internal temperature

INTRODUCTION

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Received Date: August 27, 2022

Accepted Date: September 06, 2022

Published Date: November 30, 2022

Citation: Numan Siddique Mazumder, Pradip Lingfa, Asis Giri. Effect of Initial Temperature and Diameter of Ethanol Droplet on Evaporation Dynamics in Convective Air Medium. Journal of Polymer & Composites. 2022; 10(Special Issue 1): S18–S24.

The droplet evaporation process is important in demanding engineering applications such as spray combustion, turbojet engine, air conditioning, etc. In spray combustion application, bulk liquid fuel is injected into the combustion chamber to produce smaller particles of droplets and before the combustion process starts, the droplet has to be vaporized first. Commonly fossil fuels (such as petrol and diesel) are used as a primary combustor in combustion applications. Due to the depleting reserve and environmental concerns, clean and renewable fuels are getting lots of attention now a day. Ethanol is one of the suitable alternatives among other biofuels as it has high octane numbers and low carbon emission [1]. Pure ethanol is also used as a primary fuel in auto industries in Brazil [1].

Some studies [2–4] in a stagnant ambient environment have been performed on ethanol droplets, but in the spray combustion process, a relative velocity exists between the droplet and the surrounding gas. Moreover, in a convective gaseous medium, the ethanol droplet evaporation process has been investigated by a few researchers [5–7]. Raghuram et al. [5] performed a numerical analysis of the evaporation characteristics of bi-component ethanol and methanol droplet. To capture the momentum transfer in both gas and liquid phases, they solved the Navier-Stokes equation of the spherical polar coordinate system in the finite volume method. They observed insignificant effects on droplet lifetime at various blending compositions of ethanol in the mixture. However, they have not performed any parametric studies on the initial diameter and temperature of pure ethanol droplets. For the case of pure and blended ethanol droplets, Saha et al. [6] numerically and experimentally investigated the evaporation characteristics of ethanol, but the Reynolds number was selected as low. Narasu et al. [7] developed a semi-analytical model to study the bi-component ethanol and water droplet under a force convection environment. But the model developed by them is not suitable for spray combustion application as the Reynolds number ($Re < 20$) was low.

There may be a research gap that exists in investigating the evaporation dynamics of pure ethanol droplets in the moderate Reynolds number ($20 < Re < 100$) range. This motivated us to perform this study on pure ethanol to evaluate the effects of droplet initial diameter and temperature. In this work, we have mathematically simulated the droplet evaporation process under a force-convective air environment. The droplet is floating in a hot convective medium in absence of gravity. Gas and liquid phase motion is considered along with unsteady droplet heating, variable Stefan (blowing effect) flow, and non-unitary Lewis number. The well-established conservative governing equations of species, momentum, and energy equations of spherical polar coordinates are solved in the finite difference method with appropriate boundary conditions. The flow is considered laminar, and axisymmetric and the radiation effects are negligible in the present physical scenario evaporation process.

GOVERNING EQUATIONS

For capturing the momentum transfer in both gas and liquid phases the vorticity and stream function equations of a spherical coordinate system are used, while for the energy and species transfer, the convection and diffusion equation is utilized. The non-dimensional governing equations, and initial and boundary conditions are given below [8].

The vorticity equation:

$$\left[\frac{\partial \psi}{\partial r} \frac{\partial}{\partial \theta} \left(\frac{\omega}{r \sin \theta} \right) - \frac{\partial \psi}{\partial \theta} \frac{\partial}{\partial r} \left(\frac{\omega}{r \sin \theta} \right) \right] \sin \theta = \frac{2}{\Gamma} \left[\frac{\partial^2 \zeta}{\partial r^2} + \frac{\partial \zeta}{\partial \theta^2} + \frac{\partial \zeta}{\partial r} + \cot \theta \frac{\partial \zeta}{\partial \theta} \right] \quad (1)$$

$$\zeta = \omega r \sin \theta, \quad \Gamma = Re \text{ (for gas phase)}, \quad \Gamma = Re \frac{\mu^g}{\rho^g} \frac{\rho^l}{\mu^l} \text{ (for liquid phase)}$$

The stream function equation:

$$\frac{\partial^2 \psi}{\partial r^2} + \frac{\partial^2 \psi}{\partial \theta^2} + \frac{\partial \psi}{\partial r} + \cot \theta \frac{\partial \psi}{\partial \theta} = \omega r \sin \theta \quad (2)$$

The generalized convection–diffusion equation:

$$\frac{\partial \phi}{\partial t} + \kappa \left(V_r \frac{\partial \phi}{\partial r} + \frac{V_\theta}{r} \frac{\partial \phi}{\partial \theta} \right) = \frac{2}{\Gamma} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \phi}{\partial \theta} \right) \right] \quad (3)$$

For steady temperature equation (gas phase), $\frac{\partial}{\partial t} = 0$, $\phi = T^g$, $\kappa = 1$, $\Gamma = Pe$

For steady species concentration equation (gas phase), $\frac{\partial}{\partial t} = 0$, $\phi = C$, $\kappa = \frac{Pe}{2}$, $\Gamma = \frac{0.5}{Le}$

For unsteady temperature equation (liquid phase), $\phi = T^l$, $\kappa = \frac{Pe_i^g}{2a} \frac{\alpha_i^g}{\alpha_i^l}$, $\Gamma = \frac{0.5}{a^2} \frac{\alpha^l}{\alpha_i^l}$

$$\text{Radial velocity at drop surface: } V_s = -2 \frac{\partial C}{\partial r} \bigg|_{r=1} / Re^g Sc^g (1 - C_s) \quad (4)$$

$$\text{Depletion of droplet diameter: } \frac{\partial a}{\partial t} = - \frac{\rho^g}{\rho^l} \frac{Pe_i^l}{2} \bar{V}_s \quad (5)$$

Boundary Conditions

The following boundary conditions are applied while solving the above governing equations.

$$\begin{aligned} \text{At } (r \rightarrow \infty): \psi^g &= 0.5r^2 \sin^2 \theta + \bar{V}_s (\cos \theta - 1), \omega^g = 0, T^g = T^\infty, C = 0, \text{ at } (r = 0); \psi^l = 0, \omega^l = 0, \\ \frac{\partial T^l}{\partial r} &= 0 \text{ At } (\theta = 0) \text{ \& } (\theta = \pi): \omega^g = \omega^l = 0, \frac{\partial T^g}{\partial \theta} = \frac{\partial C}{\partial \theta} = \frac{\partial T^l}{\partial \theta} = 0, \text{ at } (\theta = 0): \psi^g = 0, \text{ and at } \\ (\theta = \pi): \psi^g &= -2\bar{V}_s \end{aligned}$$

$$\text{At } (r = 1): \psi^g = \bar{V}_s (\cos \theta - 1), \psi^l = 0, \frac{\partial \psi^g}{\partial r} = \frac{\partial \psi^l}{\partial r}, \frac{\partial}{\partial r} \left(\frac{1}{r^2} \frac{\partial \psi^g}{\partial r} \right) = \frac{\mu^l}{\mu^g} \frac{\partial}{\partial r} \left(\frac{1}{r^2} \frac{\partial \psi^l}{\partial r} \right), T^g = T^l$$

$$\frac{\partial T^g}{\partial r} = \frac{k^l}{k^g} \frac{\partial T^l}{\partial r} + \frac{1}{2} Pe_i^g Kua \left(\frac{\Delta H_v}{\Delta H_{vi}} \frac{Cp_i^g}{Cp^g} \frac{\alpha_i^g}{\alpha^g} \right) V_s, \text{ and } C_s = 1 / \left(1 + \left(\frac{M^\infty}{M_v} \right) \left(\frac{P^\infty}{P_v} - 1 \right) \right)$$

Initial Conditions

$$\text{At } (t = 0): T^l = 1 \text{ for } 0 \leq r \leq 1, \text{ and } T^g = T^\infty \text{ for } r > 1$$

SOLUTION TECHNIQUE

The transport equations of the gas domain are transformed into a stretch coordinate ($r = e^z$) system to generate denser grids in the vicinity of the droplet surface. Stream function and the vorticity equations are discretized using the method of Hamielec et al. [9] and while the energy and concentration equations are discretized using Peric's [10] convection-diffusion scheme. 1st order upwind scheme is utilized for the convection term and the 2nd order central difference scheme is used for the diffusion term. The unsteady term of the energy equation of the liquid phase is discretized with Crank Nicolson Scheme. The successive over-relaxation (SOR) method is used while solving the stream function and vorticity equations and the rest of the convection-diffusion equations are solved using Stone's SIP [11] solver. The maximum radial length of the free stream location of the gas phase is kept fifty times the droplet non-dimensional radius. The number of grid points along the radial direction of the gas and liquid domains is kept at 120 and 40, respectively and for the azimuthal direction, 60 grid points are taken. The constant time step of about 0.0001 is utilized for the unsteady energy equation. The inner iterations are terminated when the relative values of consecutive iterations of any parameter fall below 10^{-6} . Outer iteration was stopped when the non-dimensional droplet radius decreases to 33% of its initial values. Thermo-physical properties of pure ethanol and air are estimated as a function of temperature using the semi-empirical co-relations [12–14] and the mixture properties are evaluated as a function of a reference temperature and concentration (1/3 rule) with appropriate mixing rules.

VALIDATION

In Figure 1, the d^2 -curve of the ethanol droplet is compared with the existing literature [2, 7, 15] at two different Reynolds numbers ($Re = 0.01$ and $Re = 68.15$). The initial aero-thermal conditions of

each case are displayed in the respective figures. In Figure 1(a), the numerically predicted d^2 -curve for quiescent ambient is compared with Pinheiro et al. [2]. Pinheiro et al. [2] have performed a semi-analytical study on an evaporation process of pure ethanol droplets to evaluate the effects of ambient temperature, free stream pressure, and ambient fuel vapor concentration. To resemble the quiescent ambient condition, we have considered a low velocity such that the Reynolds number becomes close to zero ($Re = 0.01$).

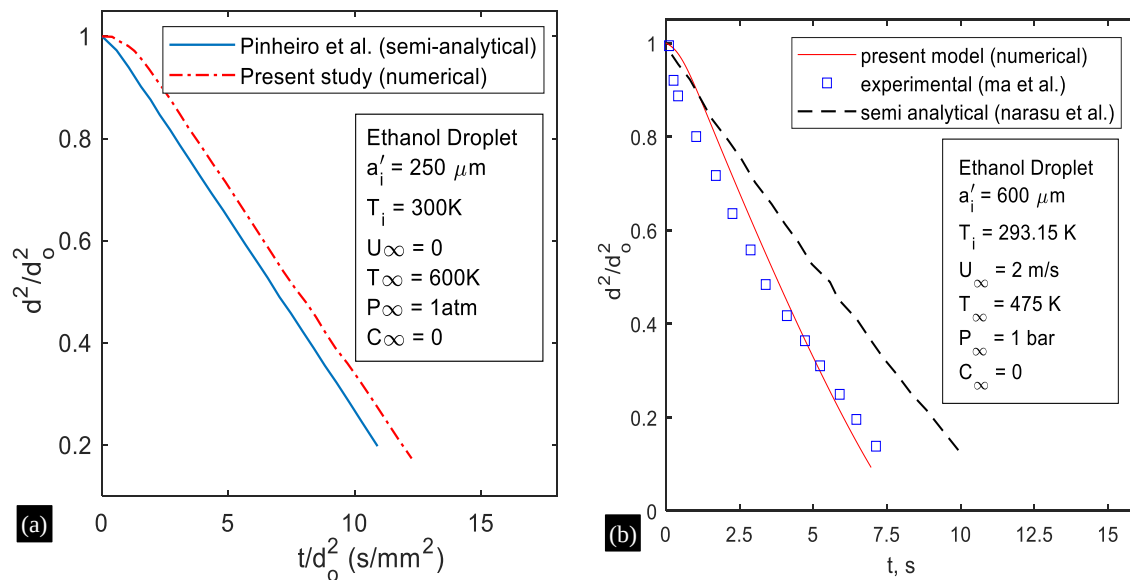


Figure 1. Comparison of d^2 -curve of ethanol droplet at (a) quiescent ambient ($Re = 0.01$), and (b) moderate Reynolds number ($Re = 68.15$) with the existing literature.

Moreover, for the case of convective air medium ($Re = 68.15$), Ma et al. [15] and Narasu et al. [7] studied the evaporation process of bi-component ethanol and water droplet at various mass fractions of ethanol. For the case of comparison, we have picked a particular d^2 -curve where they chose ethanol mass fraction to unity. It can be observed from Figure 1(b) that the d^2 -curve from our study is closer to the experimental data [15]. As our numerical model is aligned with the d^2 -curve of the existing experimental study, hence it can be concluded that the present model is accurate enough to study the natural phenomenon of the ethanol droplet evaporation process.

RESULTS AND DISCUSSION

In Figure 2(a), the temporal variation of the non-dimensional diameter square (d^2 -curve) of the ethanol droplet is shown whereas, in Figure 2(b), the temporal evolution of the droplet bulk temperature is illustrated for three different initial diameters (such as $d_o = 0.2\text{ mm}$, 0.6 mm , and 1.0 mm) at $Re = 100$ and $T_\infty = 600\text{ K}$. The initial aero-thermal conditions are also displayed in Figure 2(b). The droplet with diameter; $d_o = 0.2\text{ mm}$, 0.6 mm , and 1.0 mm have been subjected to three different free stream velocities $U_\infty = 25.7\text{ m/s}$, $U_\infty = 8.5\text{ m/s}$, and $U_\infty = 5.15\text{ m/s}$, respectively to maintain uniform $Re = 100$ at $T_\infty = 600\text{ K}$. It can be observed from Figure 2(a) that the droplet having a smaller diameter ($d_o = 0.2\text{ mm}$) evaporates early compared to the bigger droplet ($d_o = 1.0\text{ mm}$). This is occurring as smaller droplet has higher specific surface area compared to bigger droplet as it requires less energy to evaporate. Moreover, the smaller droplet is also subjected to higher ambient velocity ($U_\infty = 25.7\text{ m/s}$) compared to the bigger droplet to maintain a uniform Reynolds number ($Re = 100$). Furthermore, it is observed from Figure 2(b) that irrespective of initial diameter, the wet-bulb temperature (also called saturation temperature) of the droplet is also the same. But, the heat-up periods are different. A bigger droplet requires more heating time to reach the saturation condition compared to the smaller counterpart.

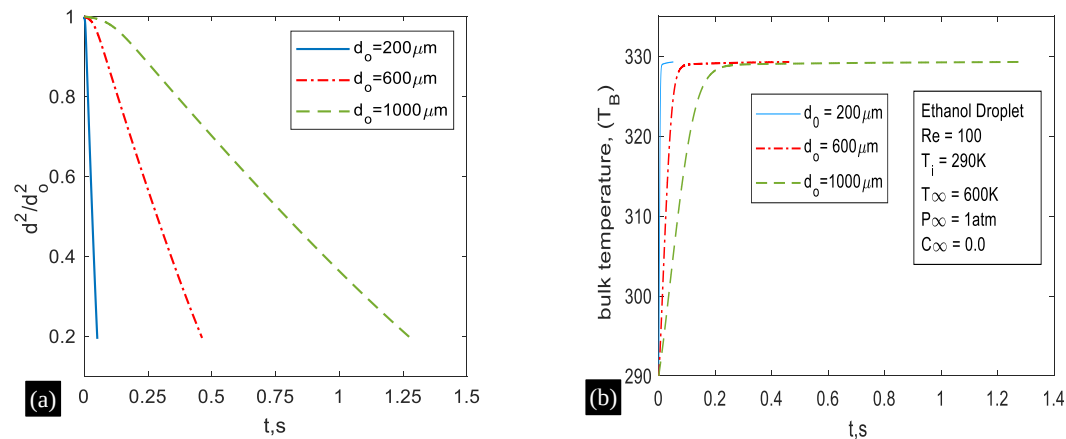


Figure 2. The temporal variation of (a) droplet diameter and (b) bulk temperature.

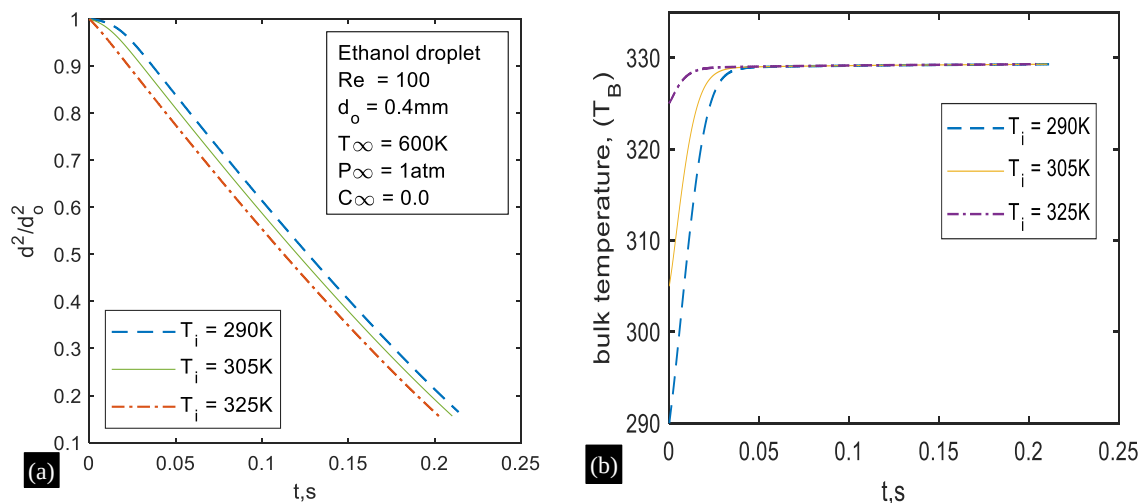


Figure 3. Temporal variation of (a) droplet diameter and (b) bulk temperature of ethanol droplet at three different initial droplet temperatures.

In Figure 3, the temporal variation of the non-dimensional diameter square and the bulk temperature of the droplet is shown for three different initial droplet temperatures ($T_i = 290, 305$, and 325 K). The initial $Re = 100$ at $T_\infty = 600\text{ K}$ is kept uniform for all cases studied. The initial aerodynamics conditions are also displayed in Figure 3(a). From the d^2 -curve plot (Figure 3(a)), it can be observed that the droplet with a higher internal temperature is evaporating a little early compared to its lower counterpart. However, the differences in droplet lifetime due to changes in internal temperature are minimal compared to the initial diameter (Figure 2(a)). Moreover, from the bulk temperature plot of Figure 3(b), it is observed that the droplet heat-up period is less for droplets having a higher internal temperature. But, in all cases, evaporation occurs at uniform wet-bulb temperature (329 K). The wet-bulb temperature recorded here from the present numerical simulation of ethanol droplets at $T_\infty = 600\text{ K}$ is also aligned with the temperature predicted by Castanet et al. [16] for ethanol droplets.

In Figure 4, the flow pattern of gas and liquid phases, and temperature and fuel vapor concentration contour plots of the gas phase of the evaporating ethanol droplet are shown at time instant $t = 0.46\text{ s}$. The droplet is evaporating in a convective hot air environment ($T_\infty = 600\text{ K}$) under zero gravity conditions. The droplet has an initial temperature $T_i = 290\text{ K}$, initial diameter $d_o = 0.6\text{ mm}$, and initial Reynolds number $Re = 100$. However, the contour plots of Figure 4 are having instantaneous Reynolds number $Re(t) = 43$ at $t = 0.46\text{ s}$. The decrease in Reynolds number is observed due to the reduction in diameter as droplet size gets reduced in the evaporation phenomenon. Also, the

corresponding instantaneous Peclet number (Pe), Lewis number (Le), and Schmidt number (Sc) are displayed in the respective figures. Typically, a vortex structure in the downstream location of a sphere is formed at $Re = 43$, however, due to the surface-blowing effect of the evaporation process, the vortex ring tends to diminish in this case. Also, from the isotherm plot in Figure 4(b), it can be observed that the profile of the thermal boundary layer is pointed towards the flow direction (left to right), and a considerable amount of temperature gradient is visible in the vicinity of the droplet surface. In addition, the fuel vapor concentration gradient also is more toward the downstream direction compared to the frontal location of the droplet.

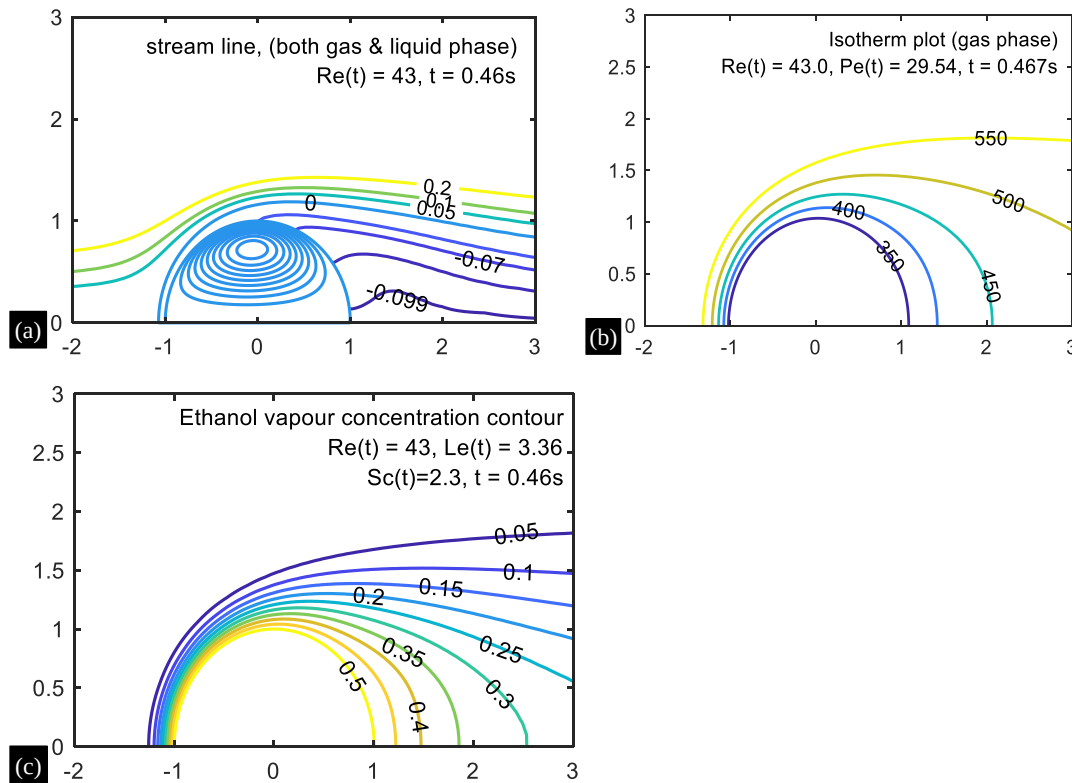


Figure 4. (a) The streamline pattern of an evaporating ethanol droplet at $t = 0.46s$, (b) The gas phase isotherm plot over an evaporating ethanol droplet at $t = 0.46s$, (c) The fuel vapor concentration plot over an evaporating ethanol droplet at $t = 0.46s$.

CONCLUSIONS

In this study, we have numerically simulated the evaporation process of an ethanol droplet in a convective air environment under zero-gravity conditions. The stream function and vorticity equation of the spherical polar coordinate system has been utilized to capture the velocity in both gas and liquid regions. The governing equations are numerically solved with the aid of the finite difference method. The present numerical work is validated by comparing the d_2 -curve of an ethanol droplet with the existing literature. Six different cases of simulations have been performed under uniform $Re = 100$ at $T_\infty = 600$ K and $P_\infty = 0.1$ MPa. Firstly, parametric studies have been performed on three different diameters ($d_o = 0.4, 0.6$, and 1.0 mm) and then, the initial droplet temperature ($T_i = 290, 305$, and 325 K) has been varied. The results reveal that the smaller droplet evaporates earlier compared to the relatively bigger droplet. The droplet heat-up period is also less for smaller droplets. A similar pattern is also observed for the initial temperature case. The droplet with a higher internal temperature has a shorter evaporation lifetime. In addition, the flow pattern in terms of streamlining, gas phase temperature profile in terms of isotherm contour, and fuel (ethanol) vapor concentration profile have been shown at time instant $t = 0.42s$. It is observed that the vortex ring at the downstream location of the evaporating droplet has diminished due to the presence of the blowing effect at the interface.

Nomenclature

a'	= droplet radius at any instant	Re	= Reynolds number, $(2U_{\infty}a'\rho/\mu^g)$
a	= non-dimensional radius of droplet, (a'/a'_i)	Sc	= Schmidt number, (ν/D_{AB})
C	= mass fraction of the liquid-vapor	Pe	= Peclet number, $(2U_{\infty}a'/\alpha^g)$
C_p	= specific heat	t	= Non-dimensional time, $(t'\alpha'_i/a_i'^2)$
D_{AB}	= Diffusivity of vapor in ambiance	μ	= viscosity
Ku	= Kutateladze number, $(\Delta H_v/C_p^l T'_i)$	ρ	= density
k	= thermal conductivity	α	= Thermal diffusivity
Le	= Lewis number	i	= at the initial stage
M	= Molecular weight	∞	= of free stream location
P_v	= Vapor pressure	d	= diameter

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