A Droplet Evaporation Model for Spray Combustion

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1 Introduction

Droplet evaporation in spray combustion is one of the controlling processes for the performance and overall combustion characteristics of liquid-fuelled combustion systems. Studying and understanding the gasification of an isolated droplet may guide the improvement of spray combustion models. Although droplet evaporation has been a classical research topic for several decades, studies dealing with droplet evaporation under ambient conditions pertinent to spray combustion applications are still lacking. For example, data for a droplet evaporating in a turbulent, hot and pressurized environment are not available. A brief literature relevant to this topic is summarized below.

Gökalp *et al*. [1] proposed a vaporization Damköhler number to explain the influence of turbulence on droplet mass transfer rate. Wu *et al*. [2] followed Gökalp's idea by investigating experimentally the effect of turbulence on the evaporation rate of a wider range of hydrocarbon fuels as well as freestream turbulence intensities, but at standard temperature and pressure conditions. They confirmed Gökalp's idea by proposing an empirical correlation expressed as $K/K_L = 0.771 Da_v^{-0.111}$, where K and K_L are the droplet evaporation rates under turbulent and laminar flow conditions, respectively. Da_v is the vaporization Damköhler number, which is defined as the ratio of a turbulence characteristic time t_t over an evaporation characteristic time t_v ($Da_v=t_t/t_v$), where $t_t=(d_0)^{2/3}/\varepsilon^{1/3}$ and $t_v=\delta_M/V_r$. δ_M and V_r are the vapour film thickness around the droplet and vapour blowing velocity, respectively [3]. Hiromitsu and Kawaguchi [4] took a step further to test the aforementioned approach (i.e. the evaporation Damköhler number). They measured the evaporation rates of several droplets including *n*-hexane, *n*-heptane, *n*-octane, distilled water and ethanol in a hot airflow having a mean velocity of 2 m/s, ambient temperature ranging between 323K and 423K, and freestream turbulence intensity (i.e. $I_\infty = u'/U_\infty$ where U_∞ is the mean velocity component and u' is the mean value of the fluctuating velocity component) that varies from 0 to 18%. Their results suggested that the vaporization Damköhler number correlation, which was proposed to predict the droplet turbulent vaporization rate, would not work when the gas temperature exceeds the droplet boiling temperature. In a very recent numerical study, Abou Al-Sood and Birouk [5] tested the aforementioned correlation under a wider ranges of freestream turbulence and temperature. Their findings confirmed that the correlation proposed in terms of an evaporation Damköhler number, as presented in [1-2] in its current form, would not work for predicting the droplet vaporization rate in a turbulent hot environment. The failure of the concept of the vaporization Damköhler number to work under hot flow conditions may be due to the limitations of the semi-empirical relations used for calculating the vaporization characteristic time. Therefore some additional studies may be needed to refine the definition of this parameter, i.e. t_v.

The focus of the present numerical study is particularly to develop a mass transfer correlation for a droplet evaporating in a turbulent, hot and pressured flow environment. The outcome of this study is indeed very important for spray combustion modeling.

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2 Methodology

Governing equations

The physical problem which consists of a hydrocarbon fuel droplet having an initial radius r_0 and an initial uniform temperature T_0 is immersed in a turbulent inert airstream of infinite expanse. The gas-phase is prescribed by its freestream mean velocity, U_∞, pressure, p_∞, temperature, T_∞, fuel mass fraction, $Y_{F\infty}$, turbulence intensity, I_∞, turbulence kinetic energy, k_∞, and its dissipation per unit of turbulence kinetic energy, ω_∞. The droplet, which is stationary and consists of a single chemical component surrounded by an inert atmosphere, remains spherical (i.e. the droplet Weber number is much less than unity) throughout the vaporization process. The governing equations for the gas phase are those of mass and momentum (i.e. Reynolds-Averaged Navier-Stokes), turbulence kinetic energy, specific kinetic energy dissipation rate, and species concentration. For the liquid phase, the governing conservation equations are those of mass, momentum and energy. Closure for turbulence terms in the gas-phase governing equations is obtained by using the shear-stress transport (SST) model [6]. Heat and mass transfer terms in the energy and species concentration equations are handled by using Jones and Launder's assumption of laminar heat and mass transfer in which a turbulent Schmidt number is introduced [10]. The freestream mean velocity components, pressure, temperature, fuel mass fraction and turbulence quantities at the inlet of the computational domain are taken as $u = U_\infty, v = 0$, $w = 0$, $p = p_\infty$, $T = T_\infty$, $Y_F = 0$, $k = k_\infty$ and $\omega = \omega_\infty$. The freestream k_∞ and ω_∞ are estimated by using the following relations $k_\infty = 1.5\left(I_\infty \times U_\infty\right)^2$ and $\omega_\infty = 10U_\infty / L$ where L is the characteristic length of the computational domain [7]. The conditions at the gas-liquid interface are obtained by coupling the conservation (momentum, energy and species) equations.

Numerical approach

The governing differential equations are integrated over discrete volumes by using finite volume method. The spherical droplet in the Cartesian grid is treated by using a blocking-off technique. The use of the blocked-off technique for studying the evaporation process of a droplet in a gaseous medium requires switching the active and inactive control volumes between the gas-phase and the liquid-phase; that is, when solving for the gas-phase, the control volumes forming the liquid-phase (droplet) are inactive and those forming the gas-phase are active. Likewise when solving for the liquid-phase, the control volumes within the liquid-phase are active and those outside, i.e. the control volumes forming the gas-phase, are inactive. For the inactive control volumes, the values of the predefined diffusion parameters preserve their values before they become inactive. Although the solution is being obtained for the entire calculation domain, which includes both the active and inactive regions, the blocked-off technique consists of assigning a large source term in the discretization equation so that the solution concerns only the active control volumes. More details can be found in Ref. [5].

The calculation domain was chosen to be a cube of 32*r*x32*r*x32*r*, where *r* is the instantaneous droplet radius. The choice of the length of the computation domain, i.e. 32*r*, is based on the suggestions of Sundararajan and Ayyaswamy [8] who demonstrated that the freestream inflow conditions into the computation domain must be taken at a distance from the droplet centre that is at least 10 times larger than the droplet radius. The computation domain is divided into control volumes and the droplet is generated at the centre of the cube. In the present analysis, the Cartesian moving grid in the calculation domain consists of 60x60x60. Since the gradients around the droplet are large, a very fine grid 40x40x40 is used in the domain of 4*r*, i.e. 2*r* from the sphere centre in all directions. This grid is chosen as a compromise between the computational time and the desired accuracy of the results.

The solution of the set of linearized algebraic equations is accomplished by using three dimensional vectorized version of SIP (Strongly Implicit Procedure) developed by Leister and Peric [9]. Iterative sweeps of the solution are continued until the imposed condition is achieved.

3 Preliminary results

Results presented in this paper concern only the effect of turbulence on a droplet evaporating in a hot environment under standard pressure conditions. Work is still in progress for the additional effect of ambient

pressure. The numerical model developed in the present study is validated by comparing its predictions with published experimental data in Ref. [2].

Droplet evaporation in a turbulent airstream at standard pressure and temperature conditions

The vaporization Damköhler number correlation proposed in [1-2] is examined. The numerical data are obtained by employing a droplet Reynolds number ranging between 56 and 186, a freestream turbulence intensity in the range between 0 and 60%, and a turbulent integral length scale assumed equal 5 times the initial droplet diameter, which is the measured average value reported by Wu et *al*. [2]. The present numerical predictions confirm that Da_v can indeed predict the droplet's turbulent evaporation rate under standard pressure and temperature conditions.

Droplet evaporation in a turbulent hot airstream

Figure 1 shows the variations of *n*-heptane and *n*-decane droplets' turbulent evaporation rates normalized by their corresponding laminar values, K/K_L, for three typical freestream temperatures, i.e. 300 K, 773 K and 1273 K. This figure reveals that increasing the ambient temperature from 300 K to 773 K and then to 1273K increases K/K_L by a maximum factor of approximately 1.66, 1.51, 1.41 for *n*-heptane and 2.15, 1.87, 1.79 for *n*-decane, respectively, when varying the freestream turbulence intensity from 0% to 60%. This suggests that the effect of turbulence on droplet lifetime tends to weaken as the freestream temperature increases. In addition, it can be observed from this figure that overall the effect of turbulence is much more pronounced at lower to moderate turbulence intensities (for approximately $I_\infty < 20$). This may be explained as follows. An increase in the droplet's surroundings temperature increases the heat transfer into the droplet, which in turn increases the molecular diffusion of the vapour. As a result the vapour residence time at the droplet surface decreases which makes less available time for turbulence to act. The Damköhler number correlation, which is discussed in the previous section, is examined at freestream temperatures higher than room temperature. The tested temperatures are 363 K, 400 K, 773 K and 1273 K. It is discovered that the corresponding Damköhler number could not be used to correlate the variation of K/K_L. As an alternative, the conventional expression, which is based on Sherwood number, is employed in the present study to develop a droplet mass transfer correlation. The best fit for the present numerical data, which is displayed in Fig.2, is found to have the following expression (with a standard deviation of 93%) $Sh_f (1+B_{M,f})^{0.7} = 2 + 0.914\,\mathrm{Re}_M^{1/2}\, Sc_f^{1/3}\left(1+1.235 I_\infty^{0.372}\right)$, where B_M, Re, Sc and I are the mass transfer number, Reynolds number, Schmidt number and turbulence intensity, respectively. The subscripts f and ∞ denote film and free stream conditions. The Sherwood number in this expression is calculated as reported in [5]. This correlation is tested over a wide range of liquid properties and freestream conditions. The liquid properties are varied by using two different fuels, i.e. *n*-heptane and *n*-decane droplets. The freestream conditions are varied by changing the freestream temperature from 300K to 1273K, turbulence intensity between 0 and 60% and the freestream mean-velocity in the range between 0.6 m/s and 2 m/s.

4 Concluding remarks

A three-dimensional numerical model is developed to assess the effect of freestream turbulence intensity on the evaporation of a single droplet exposed to a hot convective flow. The air freestream conditions and liquid properties are varied to provide a wide range of test conditions. The major findings of the present study indicate that

(i) the expression proposed in the literature which correlates the effect of turbulence on the droplet vaporization rate (K/K_L) in terms of a vaporization Damköhler number (Da_v) is found to be valid only at ambient temperatures that are much below the boiling point, and

(ii) (ii) a droplet mass transfer correlation based on Sherwood number is proposed to account for the freestream turbulence effect on the mass transfer from a droplet exposed to a hot airflow.

Finally, the mass transfer correlation proposed in the present study is under examination for validation at elevated ambient pressure conditions.

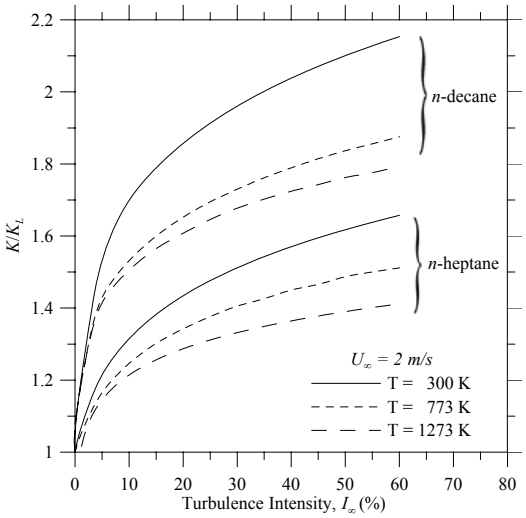

Fig. 1. K/K_L versus the freestream turbulence intensity at a typical mean velocity U_∞ = 2 *m/s* and various freestream temperatures

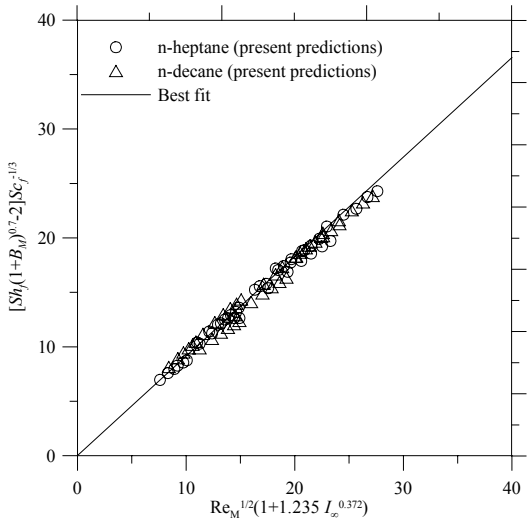

Fig. 2. Droplet's turbulent mass transfer correlation

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