

Micro-Explosion Modeling of Biofuel-Diesel Blended Droplets

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ABSTRACT

Recently, with the increasing interest on some potential alternative substitutes of petroleum fuels such as biodiesel and butanol, more and more researches are focused on the field of bio-fuels because they are renewable and friendly to the environment and can possibly reduce domestic demand on foreign petroleum. Bio-fuels are generally used in the commercial market by mixing with petroleum-based diesel or gasoline. Since the volatilities and boiling points of ethanol/butanol and diesel/biodiesel fuels are significantly different, micro-explosion can be expected in the blend mixture. In this study, a numerical model of micro-explosion including bubble generation, bubble expansion, and final breakup for multi-component bio-fuel droplets is proposed. From the simulated results of droplet characteristics at the onset of micro-explosion, it is concluded that micro-explosion is possible under engine operation condition for ethanol/butanol-diesel/biodiesel fuel blends. There exists an optimal droplet size and ambient condition for the occurrence of micro-explosion.

INTRODUCTION

The concept of micro-explosion was first presented by Ivanov in 1965 [1]. The occurrence of micro-explosion is due to the vaporization of two or more liquid components with different volatilities in a high temperature environment. Because of the finite mass diffusion velocity within the droplet, lighter components inside the multi-component droplet cannot emerge to the surface sufficiently fast to compensate its fast vaporization rate than the rest of components, and thus the mass fraction of light components inside the droplet is larger

than that at the droplet surface. As a consequence, even though the droplet surface does not pass the boiling state, the temperature in some region within the droplet is likely to be higher than the local boiling point. When the temperature is high enough to support the nucleation, one or two bubbles are generated inside the droplet. Their subsequent rapid growth results in a violent explosion of the droplet [2]. The size of the secondary droplets generated by micro-explosion is decreased significantly. From the practical viewpoint, the possible occurrence of micro-explosion has potential for making fuel atomization more flexible. That is, fine atomization does not need to be the primary concern in the design of the spraying devices and processes. In fact, it may be advantageous to have somewhat larger droplet, which possess sufficient inertia to penetrate the combustor interior in order to achieve optimal charge distribution. Upon penetration rapid gasification can then be effected through micro-explosion.

Extensive experimental studies have been done to understand the vaporization and combustion behaviors of isolated droplets in micro-explosion conditions. Micro-explosion of freely falling droplets has been experimentally observed for both miscible fuel mixtures [3,4,5], as well as water/oil emulsions [6]. Its occurrence has also been inferred from measurements of the droplet size distribution in combusting water/oil emulsion sprays [7]. Wang and Law [4] conducted a series of micro-explosion experiments using alcohol-alkane mixtures under elevated pressures. It is reported that alcohol/diesel blends can potentially enhance atomization in diesel engine due to micro-explosion. Numerical models are proposed to describe the mechanism of micro-explosion for water in fuel emulsions [8,9,10]. Most studies in micro-

Table 1. Selected thermo-physical and chemical properties for ethanol, soybean biodiesel and tetradecane

	Ethanol	Butanol	Biodiesel	Tetradecane
Density [kg/m^3] (298 K)	789.3	810.0	885.0	759.6
Boiling Point [K]	351	400	627	527
Heat of Vaporization [kJ/kg]	841	430	320	243
Viscosity [$\text{g/cm}\cdot\text{s}$] (313 K)	0.009	0.030	0.040	0.017
Surface Tension [dyne/cm] (293 K)	23.1	24.9	32.5	26.8
Vapor Pressure [mm_{Hg}] (353 K)	675.1	6.7	~ 0	2.775

explosion focused on the effects of pressure, composition, temperature, initial droplet size, internal phase structure of emulsified droplets and gravity on micro-explosion [4, 8,9,10]. Some papers studied the superheat limit, which accounts for the onset of micro-explosion [10, 11]. However, few works investigated the breakup process and the consequent outcomes before the year 2000. Based on a linear stability analysis, Zeng and Lee [2, 12] suggested a model describing the instability of micro-explosion and proposed a breakup criterion for the determination of the averaged size and velocity of secondary droplets.

Recently, some potential alternative substitutes of petroleum fuels, such as biodiesel, ethanol, and butanol, have received much attention because they are renewable and friendly to the environment [13] and can possibly reduce domestic demand on foreign petroleum. Bio-fuels are generally mixed with petroleum-based diesel or gasoline in the commercial market. Selected thermo-physical and chemical properties of ethanol, butanol, soybean biodiesel, and tetradecane are tabulated in Table 1. Since the volatilities and boiling points of ethanol and diesel/biodiesel fuels are significantly different, micro-explosion can be expected in binary mixtures of ethanol-diesel or ethanol-biodiesel. Although butanol has a higher boiling point compared to ethanol, the differences between butanol and biodiesel are still significant so that micro-explosion in binary mixtures of butanol-biodiesel might occur. Additionally, the use of a higher alcohol, like butanol, could solve the problem of fuel instability at low temperature because of the higher solubility of butanol in diesel/biodiesel fuels. Understanding the atomization process and dynamics of secondary droplets in bio-fuel and diesel blends due to micro-explosion is helpful in optimizing bio-fuel engine performances.

In this study, the effects of ambient pressure, ambient temperature, composition, and initial droplet size on the onset of micro-explosion in bio-fuel and diesel blends are examined. Atomization is determined by the aerodynamic disturbances in previous works [2, 12]. A proposed breakup model based on surface energy of droplet is used in this study, which reaches the same results in previous works [2, 12]. The droplet breakup characteristics due to micro-explosion are studied under engine operation conditions.

Numerical works are carried out by using a modified KIVA-3V Release 2 code, developed by the Los Alamos National Laboratory [14]. The thermodynamic properties of soybean biodiesel are calculated from BDProp [15] and inserted into the KIVA fuel library. BDProp is a program which can predict the properties of various types of biodiesel from their chemical structure over a range of temperature by estimating the properties of the individual methyl esters that comprise biodiesel and using mixing rules to determine the properties of the biodiesel itself. The calculated results of properties such as vapor pressure, density, enthalpy, latent heat of vaporization, surface tension, and liquid viscosity are listed according to temperature, with a value for every 10 degrees Kelvin. According to Yuan [15], the difference in boiling point of soybean biodiesel caused by composition variation in fatty acid composition is less than 5 degrees Kelvin (625.8 K - 630.3 K), so it is acceptable to choose a single point 627 K as the boiling temperature for soybean biodiesel in this study.

MATHEMATICAL FORMULATIONS

The proposed model describes the three crucial steps of micro-explosion in a droplet: bubble generation, bubble growth and breakup. The homogeneous nucleation theory [11] is used to calculate the generation of bubble within the droplet. After bubble generation, the modified Rayleigh equation is used to describe bubble growth [16]. Finally, the breakup process is modeled using a surface energy approach, which predicts the characteristics of the bubble and droplet at breakup. The Sauter mean radius (*SMR*) of secondary droplets after breakup can be calculated from the breakup model. This study primarily focuses on small droplet atomization under micro-explosion and presents a simple approach to estimate the *SMR*.

BUBBLE GENERATION

Under the assumption of spherical symmetry, a bubble with radius R_b is assumed to be formed in the center of a droplet with radius R_s , according to the homogeneous nucleation theory shown in Figure 1. Zeng [12] provides the detailed thermodynamic description of the bubble-droplet system. Based on homogeneous nucleation theory, nucleation is arisen from thermal fluctuation and intermolecular interaction

[17]. There is neither dissolved gas nor impurity within the bubble-droplet system acting as nucleation site. As a result, homogeneous nucleation requires a higher superheat limit [12]. Avedisian and Glassman [11] proposed a semi-empirical homogeneous nucleation rate formula shown in Eq. (1),

$$J = \Gamma n_0 k_f \exp\left(-\frac{\Delta A^*}{kT}\right), \quad (1)$$

where J (1/time-volume) is the nucleation rate; Γ , the probability of nucleation; n_0 , the number density; k_f , the gas collision frequency; and A^* is the activation energy. The mathematical descriptions of parameters in Eq. (1) can be found in [11]. The current work uses unity for Γ as in previous studies [2, 11, 12, 18], which allows accurate prediction, relative to experimental measurements of the superheat limit.

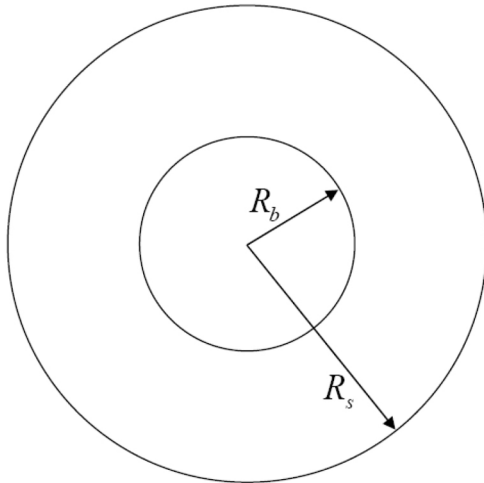


Figure 1. Bubble-droplet system

The number of nuclei can be calculated by integrating Eq. (1) with respect to time over the control volume [2]. The onset of micro-explosion, which signifies the instant of bubble generation, is determined by setting the number of nuclei to one. The exponential form on the nucleation rate indicates the drastic growth of the number of nuclei once the droplet temperature approaches the superheat limit. Therefore, the choice of the number of nuclei is insignificant in the determination of the onset of micro-explosion.

The primary concern of using homogeneous nucleation theory is that heterogeneous nucleation, due to the existence of impurity or dissolved gas, is likely to take place in practice. However, the temperature at which heterogeneous nucleation happens is bounded by the superheat limit and the saturation temperature [19, 20]. In other words, heterogeneous nucleation is possible if the droplet temperature is between these two limits. At high ambient

pressure, the superheat limit and the saturation temperature approach each other [2, 11, 12, 18]. This justifies the use of homogeneous nucleation theory in determining the nucleation temperature at high ambient pressure.

After bubble generation, the initial radius of the bubble nucleus is given by the Young-Laplace equation,

$$R_b^* = \frac{2\sigma}{P_g - P_l}, \quad (2)$$

where σ is the surface tension, P_g is the gas pressure in the bubble, P_l is the liquid droplet pressure, and R_b^* is the initial radius of the bubble. Eq. (2) addresses the mechanical equilibrium between the bubble and liquid droplet [16].

BUBBLE GROWTH

The modified Rayleigh equation describes the bubble growth process [16, 21],

$$\rho_l \left[R_b \frac{d^2 R_b}{dt^2} + 1.5 \left(\frac{dR_b}{dt} \right)^2 \right] = P_g - P_l - \frac{2\sigma}{R_b}, \quad (3)$$

where ρ_l is the liquid droplet density. The above equation states that pressure work across the gaseous-liquid interface ($r = R_b$ in Figure 1) is converted into kinetic energy, the two terms on the left hand side and surface energy, the last term on the right hand side. Note that dR_b/dt is the bubble expansion velocity. Some studies add viscous terms into the Rayleigh equation to account for the viscous effect during bubble expansion. Robinson and Judd [16] showed that viscous effect is negligible compared to other terms throughout the parameter space in that study. Eq. (3) is derived by assuming the bubble expanding in an infinite medium and thus excludes the finite size effect of the medium. Additional works will be needed to extend Eq. (3) for a finite medium. In this study, the modified Rayleigh equation is mainly used to characterize the bubble expansion rate. It also gives the estimation of the Weber number at droplet surface in a small bubble-droplet system.

SAUTER MEAN RADIUS OF SECONDARY DROPLETS

Consider a bubble-droplet system with bubble radius R_b , droplet surface radius R_s , and bubble expansion rate (V_b), written as dR_b/dt in Eq. (3), at the instant of breakup; the SMR of the secondary droplets can be obtained from conservation equations, assuming the system is spherical symmetric as in [18]. Previous work [12] assumes the secondary droplets are Chi-squared (χ^2) distributed. Current model extends previous derivation [12] by describing the size distribution of the secondary droplets using a generic