



## Research Paper

## A new puffing model for a droplet of butanol-hexadecane blends

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## HIGHLIGHTS

- A puffing model including surface evaporation, bubble growth and bubble breakup processes was developed.
- The Rayleigh equation was modified to simulate the bubble growth inside a small droplet.
- The developed model well simulated the three phases of the puffing process of a BUT50 droplet.
- The turning point of temperature curve was simulated when droplet diameter had the strong fluctuation.

## ARTICLE INFO

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## ABSTRACT

A new model was developed to investigate the puffing process of a butanol-hexadecane droplet. The puffing model took into account all the key processes, including the surface evaporation, bubble formation, bubble growth and bubble breakup. The Rayleigh equation was modified to simulate the bubble growth inside a small droplet. The sub-models for surface evaporation and bubble growth were firstly verified against the previous experimental data. Then the droplet puffing experiments of butanol-hexadecane blends were conducted under 1 bar and 750 K condition using the droplet suspension technique to further verify the puffing model. Results showed that the puffing model well simulated three phases of BUT50 (50% butanol and 50% hexadecane by mass). The three phases were the transient heating, fluctuation evaporation and equilibrium evaporation phases. An extremely strong fluctuation and several weak fluctuations were observed during the fluctuation evaporation phase from the experimental normalized squared diameter. Due to the model hypotheses, these weak fluctuations were ignored and only the strong fluctuation was simulated in the present model. Furthermore, a significant turning point was observed in the experimental temperature curve when the droplet diameter had the strong fluctuation. The occurrence of the strong fluctuation was caused by the obvious bubble expansion inside the droplet. The numerical results showed that the significant heat absorption for the bubble expansion led to the turning point in the temperature curve.

## 1. Introduction

The concerns of environmental protection and fossil fuel depletion have made the clean and sustainable energy sources more popular globally. Alcohols, as oxygenated renewable fuels, are regarded as promising alternative fuels for transportation [1]. Comparing with methanol and ethanol, butanol has higher energy density and better miscibility with diesel [2]. The addition of butanol into diesel changes the combustion and emission characteristics of an engine due to its very different physical properties from diesel [3]. The combination of butanol addition and exhaust gas recirculation (EGR) can break through the tradeoff between  $\text{NO}_x$  and soot emissions [4]. The oxygen content in butanol can bring more oxygen into the fuel-enriched area to reduce

soot emissions. The addition of butanol can result in puffing or micro-explosion phenomenon [5] and further enhance the fuel-air mixing process. This is because the boiling point of butanol (390.7 K) is significantly lower than that of diesel (555–611 K) [3]. Therefore, it is important and meaningful to study the puffing mechanism of butanol-diesel blends. However, it is difficult to investigate the puffing mechanism using diesel due to its multi-components. Hexadecane can be regarded as a representative for diesel and therefore used as the test fuel in this work [6]. In the present study, both experiments and simulations were conducted to investigate the puffing mechanism of a butanol-hexadecane droplet.

In droplet experiments, two commonly employed techniques are the droplet suspension technique and the freely falling technique [7]. The

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**Nomenclature**

A	area [m <sup>2</sup> ]
B <sub>M</sub> , B <sub>T</sub>	spalding mass and heat transfer number [-]
c	specific heat capacity [J/(kg K)]
D	binary diffusion coefficient [m <sup>2</sup> /s]
d	diameter [m]
e	the fraction of evaporation rate [-]
F	source flow strength [m <sup>3</sup> /s]
h	specific enthalpy [J/kg] or convective heat transfer coefficient [W/(m <sup>2</sup> K)]
J	mass flux [kg/(m <sup>2</sup> s)] or the nucleation rate [1/(m <sup>3</sup> s)]
k <sub>B</sub>	Boltzmann constant [J/K]
M	molar mass [kg/mol]
N	number of active nuclei [-]
Nu	Nusselt number [-]
P	pressure [Pa]
Pr	Prandtl number [-]
q	heat flux [W/m <sup>2</sup> ]
R	distance from the center of the droplet [m]
$\dot{R}$	velocity at the boundary of control volume [m/s]
$\ddot{R}$	acceleration at the boundary of control volume [m/s <sup>2</sup> ]
Re	Reynolds number [-]
S	surface tension [N/m] or source term in the energy equation [W/m <sup>3</sup> ]
Sh	Sherwood number [-]
Sc	Schmidt number [-]
t	time [s]
T	temperature [K]
u	radial velocity [m/s]
V	volume [m <sup>3</sup> ]
X	molar fraction [-]

Y	mass fraction [-]
$\rho$	density [kg/m <sup>3</sup> ]
$\varepsilon$	emissivity [-]
$\lambda$	thermal conductivity [W/(m K)]
$\mu$	dynamic viscosity [Pa s]
$\sigma_{rr}$	normal stress [Pa]
$\sigma$	Stefan–Boltzmann constant [W/(m <sup>2</sup> K <sup>4</sup> )]
$\nu$	kinematic viscosity [m <sup>2</sup> /s]
$\omega$	disturbance growth rate [1/s]

**Subscripts**

b	adjacent to bubble surface in the liquid phase
B	inside the bubble
con	convection
d	adjacent to droplet surface in the liquid phase
dif	diffusion
g	ambient gas around droplet surface
i	individual component
jun	thermocouple junction
l	liquid phase
n	total number of species
p	constant pressure
radia	radiation
s	adjacent to droplet surface in the ambient gas
sat	saturation condition
therm	thermocouple
v	fuel vapor
wir	thermocouple wire
+, -	two boundaries of control volume
$\infty$	at infinity

droplet suspension technique was widely used to verify the evaporation and puffing models because droplet images and temperature could be easily obtained [8,9]. The ambient temperature, pressure and fuel composition can influence the puffing strength. Ma et al. [10] studied the evaporation and puffing characteristics of acetone-butanol-ethanol (ABE) and diesel blends under different ambient temperatures. The results showed that the puffing strength increased with the increase of ambient temperature. Ghassemi et al. [11] studied the evaporation and puffing characteristics of heptane-hexadecane blends at elevated pressures and temperatures. The results showed that high ambient temperature and low ambient pressure would enhance the puffing phenomenon. Hoxie et al. [12] investigated the puffing and combustion behaviors of soybean oil-butanol blends including BUT00, BUT25, BUT40, BUT50 and BUT75. BUT25 represented the blend of 25% butanol and 75% soybean oil by volume in this paper. The results showed that BUT40 exhibited the most violent puffing among all the test fuels. Avulapati et al. [13] studied the puffing and micro-explosion characteristics of diesel–biodiesel–ethanol blends. Micro-explosion was defined as the phenomenon that a whole parent droplet disintegrated into smaller droplets. Puffing was defined as the phenomenon that the explosion was limited to a portion of the parent droplet [13,14]. In general, the intensity of micro-explosion was higher than that of puffing. Micro-explosion phenomenon was only observed in the ternary blends within the ethanol percentage of 10–40% while puffing phenomenon was observed beyond this range. The free-falling technique could eliminate the influence of suspension wire. However, the droplet was surrounded by the visible flame in the free-falling technique because the droplet was ignited by a flat-flame burner [15,16]. The combustion led to quick droplet heating and surface evaporation. The focus of this work was the puffing process, in which the combustion model was not contained. To the best of the authors' knowledge, no publications could

be found for pure puffing process using the free-falling technique. Therefore, the puffing model could not be verified by the free-falling technique at the present.

As reviewed above, the majority of puffing studies were conducted using experimental methods. However, a few works on the puffing model were reported due to the complexity of puffing process. Watanabe et al. [17] considered the unsteady puffing of emulsified fuel as a continuous phenomenon to apply the puffing model for the simulation of spray combustion. Ra et al. [18,19] and Zuo et al. [20] studied a vaporization model for the flash boiling. Bubble formation and growth were ignored in their models. The effect of bubble disturbance in a droplet was considered as the enhanced heat transfer from droplet inner to droplet surface. Zeng et al. [21,22] studied the breakup process of the droplet-bubble system by linear instability analysis. Bubble growth in a droplet would cause unstable waves on the bubble and droplet surfaces. The breakup was supposed to occur when the amplitude of disturbance wave grew larger than the difference between the droplet and bubble radiuses. The evaporation process on the droplet surface made no difference on bubble growth in their model. Chang et al. [23] simplified the bubble growth process for flash boiling without computational grids. Many shortages could be found in the above reviewed numerical studies. Firstly, bubble growth inside the droplet was not contained in the models of Ra et al. [18,19] and Zuo et al. [20]. Secondly, evaporation process on droplet surface was not considered in the model of Zeng et al. [21,22]. Finally, it was inaccurate to assume that bubble growth was in an infinite domain of liquid [21–23].

In this paper, a new puffing model including the bubble formation, bubble growth, bubble rupture and surface evaporation was developed. The sub-models for surface evaporation and bubble growth were firstly verified against the previous experimental data. Then, droplet puffing

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