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Multi-phase flow-I
Mon. Jul 15, 2024 10:45 AM - 12:45 PM Room D

[1-D-02] Numerical simulation of enhanced evaporation by puffing bi-component droplet

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Twelfth International Conference on Computational Fluid Dynamics (ICCFD12), Kobe, Japan, July 14-19, 2024

Numerical simulation of enhanced evaporation by puffing bi-component droplet

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Abstract: In this study, the break-up of a bi-component droplet comprising miscible species and containing a fuel vapor bubble, through the puffing phenomenon is investigated using three-dimensional (3D) numerical simulations employing the Coupled Level-Set and Volume Of Fluid (CLSVOF) method for interface capturing. Specifically, the effect of the ambient pressure on the droplet's puffing, evaporation, and fuel vapor spreading behavior is analyzed in detail. The results show that puffing consists of the fundamental phenomena of ligament formation and fragmentation, and vapor ejection from the bubble, which promote evaporation of the fuel and vapor spreading. In addition, these effects are suppressed under higher ambient pressure conditions.

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1 Introduction

It is known that droplets of such multi-component liquid fuels during the evaporation process can cause secondary atomization by phenomena called puffing and micro-explosion [1]. However, numerical studies on the puffing phenomenon of multi-component droplets containing miscible species are extremely limited. One example being the 3D numerical analysis of puffing in bi-component droplets comprising a miscible mixture of butanol and tetradecane performed by Guida et al. (2022) [2]. While they investigated the puffing dynamics of these bi-component droplets by using the Coupled Level-Set and Volume of Fluid (CLSVOF) method [3, 4], they did not discuss the processes such as fuel evaporation and the subsequent spreading of fuel vapors in their study. This is mainly due to the difficulty in accurately reproducing the evaporation behavior of droplets with miscible components.

Therefore, this study aims to investigate the break-up of a bi-component droplet composed of miscible species of n-heptane and n-hexadecane and containing a fuel vapor bubble, through the puffing phenomenon using 3D numerical simulations employing the CLSVOF interface capturing method. Specifically, the effect of the ambient pressure on the droplet's puffing, evaporation, and fuel vapor spreading behavior is examined in detail.

2 Numerical Methods and Configurations

For both the gas and liquid phases, the governing equations for the conservation of mass, momentum, enthalpy, and chemical species are solved. These equations are solved taking into account the discontinuity at the gas-liquid interface [5, 6] and the evaporation rate is calculated assuming boiling evaporation. The Coupled Level-Set and Volume of Fluid (CLS-VOF) method is used to capture the gas-liquid interface in which the advection equation of the VOF function is solved and the Level-set function is calculated from the VOF function to capture the interface accurately and the Piecewise Linear Interface Calculation (PLIC) scheme [7, 8] is used for the interface reconstruction.

As specific computational configurations, the initial mass fractions of the gas phase are 77 % nitrogen and 23 % oxygen, simulating an atmosphere, the ambient temperature is 650 K, and the ambient pressure is 0.1 MPa. The initial mass fractions of the droplet's components are 50 % n-heptane and 50 % n-hexadecane, the initial droplet temperature is 466 K, and its initial diameter is 1.2 mm. The initial mass fraction of the vapor inside the bubble is 100 % n-heptane, the bubble's initial temperature is as same as that of the ambient, i.e., 650 K, and its initial diameter is 0.3 mm. A case without bubble

is also provided for comparison of evaporation rates. The computational domain is a 3.6 mm × 2.4 mm× 2.4 mm rectangular region, and the computational grid is a uniform orthogonal staggered grid with 20 μm spacing.

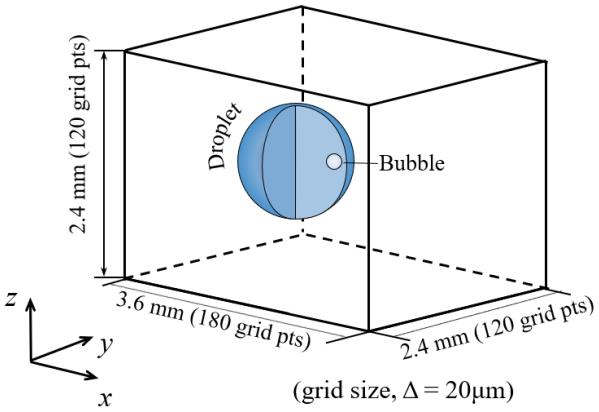

Figure 1: Schematic of computational domain and initial settings.

Table 2: Summary of calculated cases.

Case	Ambient Pressure [MPa]	Droplet Diameter [mm]	Bubble Diameter [mm]
P01A	0.1	1.2	0.3
P01B	0.1	1.2	-
P05A	0.5	1.2	0.3
P05B	0.5	1.2	-
P10A	1.0	1.2	0.3
P10B	1.0	1.2	-

3 Results and Discussion

Figure 1 shows the moment after puffing in case P01A (with fuel bubble). The fragmented liquid ligament generated after the break-up of the bubble, producing some small secondary droplets. Fig. 2 shows the comparison of total evaporation rate of *n*-heptane in case P01A (with fuel bubble) and P01B (without fuel bubble). In case P01A, the total evaporation rate remains higher after around the moment when puffing occurs (t = 0.5 [ms]) than in case P01B, where there are no bubbles and puffing is not induced. These results indicate a clear contribution of puffing to evaporation process. This is because the ligament and secondary droplets created by puffing exit from the low-temperature boundary layer in the vicinity of the mother droplet and are exposed to high temperatures ambient air, resulting in enhanced evaporation.

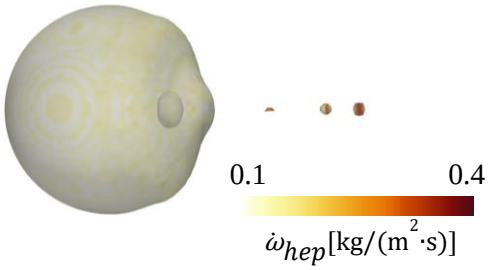

Figure 2: Distribution of *n*-heptane evaporation rate on the vapor-liquid interface in case P01A ($\boldsymbol{t}$ = 1.10 [ms]).

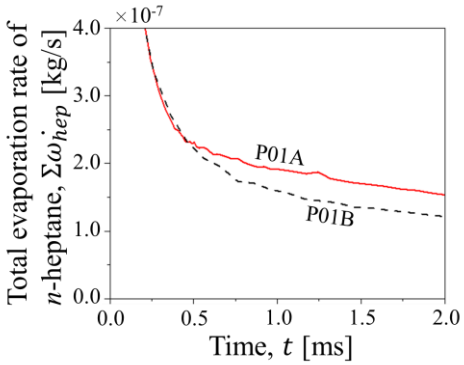

Figure 3: Comparison of total evaporation rate of *n*-heptane in case P01A (with fuel bubble) and P01B (without fuel bubble).

4 Conclusion and Future Work

In this study, the break-up and evaporation behavior of a bi-component droplet composed of miscible species (*n*-heptane and *n*-hexadecane) and containing a fuel (*n*-heptane) vapor bubble, through the puffing phenomenon was investigated using 3D numerical simulations. As a result, it was confirmed that small secondary droplets generated by puffing promotes the evaporation of fuel.

Acknowledgement

This work was supported by JST, the establishment of university fellowships towards the creation of science technology innovation, Grant Number JPMJFS2123.

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