

A Computational Study of Micro-Droplet Dynamics in Water-Oil Emulsion Droplets

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Abstract

The dynamics of a micro-droplet in a water-oil emulsion droplet were numerically studied to identify the physical mechanism for the experimentally observed behavior that the component in the dispersed micro-droplets always vaporizes first. This phenomenon was observed regardless of the types of emulsion droplets, and the mechanism has not been clearly understood. An Eulerian-Lagrangian method was implemented with a temperature-dependent interfacial tension model in order to effectively capture the thermo-capillary effect of a micro-droplet. The present study confirms that the Marangoni effect is the key mechanism to drive the micro-droplets to the emulsion droplet surface at higher temperature for both water-in-oil and oil-and-water emulsion droplets.

Introduction

The combustion characteristics of emulsion fuel droplets are attractive due to its rapid combustion and low emission benefits. The secondary atomization by micro-explosion induces a rapid explosive evaporation from the interior of emulsion droplets, therefore improves combustion efficiency with enhanced air-fuel mixing and reduced total combustion time. Furthermore, the addition of water suppresses the production of pollutant emissions such as unburned hydrocarbons, nitric oxides, and soot due to OH radical production and reduced flame temperature.¹

Two limiting models of such a multi-component droplet combustion were proposed based on the relative volatilities and concentrations of water and oil, the intensity of internal circulation, and the immiscibility.^{1,2} In the distillation limit, there is an intensive internal circulation such that the droplet interior can be approximated as being spatially homogeneous but varying only temporally due to vaporization on surface. In the slowest frozen limit, on the other hand, there is no movement inside emulsion droplet, thus the droplet composition can be assumed to remain as their initial composition.² However, the practical emulsion droplet combustion is neither homogeneous nor steady unlike these limiting models.

A number of studies have been focused on the micro-explosion itself of emulsion droplets due to the improved combustion efficiency followed by secondary atomization.^{3,4} For the evaporation process of emulsion droplet, Chung and Kim reported an interesting phenomenon by experimental study, where the component consisting of the micro-droplets always vaporizes first.⁵ A strong mechanism of transporting micro-droplets to the vaporizing emulsion droplet surface was expected, but the mechanism has not been clearly understood.

In order to understand the physical mechanism of these phenomena, high-fidelity computational studies are required due to the difficulties in detailed experimental measurements of small micro-droplets physics in an emulsion droplet. The oil and water in

emulsion droplets are immiscible each other and have different material properties. Therefore multiphase modeling should be considered with moving surface tracking and interfacial dynamics modeling including interfacial tension and steep jump in material properties.

Tracking the moving interfaces between different phases is the most critical requirement in multiphase computation because interfacial tension computation is directly related to the interface geometry. Interface tracking methods can be categorized in three groups; Eulerian, Lagrangian, and Eulerian-Lagrangian method.⁶ Eulerian methods uses a scalar function in stationary grids to extract interface location, and have been commonly used in favor of its simplicity, but the accuracy is limited due to the implicit tracking of the interface via post-processing of a scalar function in a cell. The Lagrangian method is most accurate because the interface can be represented directly on its body-fitted grid, but maintaining satisfactory grid quality remains a challenge, especially when large deformation takes place. The Eulerian-Lagrangian method utilizes a separate set of Lagrangian moving meshes representing the interface on a stationary Eulerian grid to compute the flow fields.^{7, 8} The interface can be represented accurately due to explicit interface tracking by surface meshes, and it does not require modifications to the computational grid. It is known that the interface tracking and interfacial tension computations are more accurate and efficient in Eulerian-Lagrangian method than Eulerian method at the same level of grid resolutions.^{8,9} Sim et al. implemented successfully this Eulerian-Lagrangian method for modeling of a droplet evaporation by local heating and showing the fuel vapor jet ejection induced by Marangoni effect.¹⁰

In the present study, as a simplified numerical modeling, a 2-D cylindrical micro-droplet movement in an emulsion droplet with velocity and temperature gradient was simulated in a 2-D computational domain by implementing the Eulerian-Lagrangian method¹⁰ with a temperature-dependent interfacial tension model. The micro-droplet movement mechanism, in which micro-droplets always move to surface and vaporize

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Table I. Material properties of n-decane and water at 373.12 K at 0.1 MPa.

	n-decane (liquid)	water
Density ρ (kg/m ³)	667.464	958.367
Viscosity μ (kg/m·s)	3.63453×10^{-4}	2.181818×10^{-4}
Specific heat capacity C_p (J/kg·K)	2.493×10^3	4.216×10^3
Thermal conductivity k (W/m·K)	0.110943	0.679084
Interfacial tension ρ (N/m)	0.040 ($\sigma_T = d\sigma/dT = -0.00007$ N/m·K)	

first, was investigated by analyzing the interfacial dynamics around a micro-droplet. Furthermore, the comparison of micro-droplet physics between water-in-oil and oil-in-water emulsion droplets was conducted.

Problem Configuration

Figure 1 shows an example of a water-oil emulsion droplet levitated on a hot surface. The emulsion droplet is heated from the hot surface at the bottom and the shear stress, exerted at the droplet surface by external vaporized gas flow and Marangoni effect, creates a strong inner circulation. The micro-droplets circulate along the Hill's vortex in an emulsion droplet.

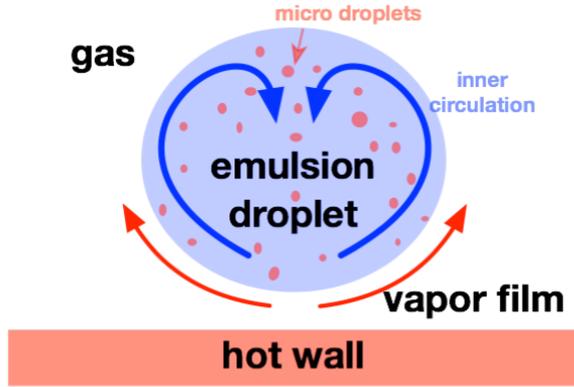


Figure 1. Illustration of an evaporating emulsion droplet levitated on a hot surface.

For a high fidelity modeling, a simplified model problem to represent a single micro-droplet in a small region of $40 \mu\text{m} \times 40 \mu\text{m}$ near an emulsion droplet surface is considered in Fig. 2. The Hill's vortex in an emulsion droplet and heat transfer from the evaporating surface is simplified by assuming constant velocity- and temperature-gradient. As a preliminary simulation, a 2-D computation was conducted with a cylindrical micro-droplet. The surface temperature is assumed 373.12 K, which is the boiling temperature of water at the given pressure of 0.1 MPa. A gravitational acceleration is ignored here because its influence on the micro-droplet can be negligible when the density difference of emulsion droplet components is small. The material properties of n-decane and water are summarized at the boiling temperature of water at 0.1 MPa in Table I.

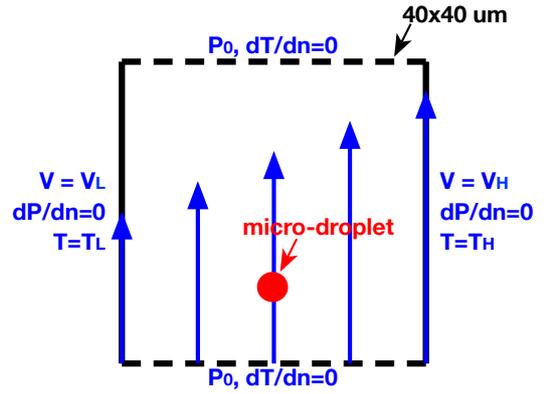


Figure 2. Illustration of a simplified numerical configuration.

Numerical Method

The objective of this study is to understand the physical mechanism for the experimentally observed behavior⁵ that the component in the dispersed micro-droplets always vaporizes first, for both oil-in-water and water-in-oil emulsion droplets. The evaporation of an emulsion droplet is fundamentally multicomponent and multiphase chemical systems. However, it has not been studied well with its multiphase interfacial dynamics characteristics. A marker-based Eulerian-Lagrangian method⁹ is implemented with a temperature-dependent interfacial tension model to model the thermo-capillary effect in an emulsion droplet. The numerical algorithm utilizes the moving Lagrangian surface meshes to treat the phase boundaries and the stationary Eulerian grids to describe the flow field. The method is chosen in favor of its accurate interface representation and explicit interface tracking. Capturing the interface geometry is very important because it determines the accuracy of interfacial tension computation and the associated convective flow and heat transfer.

The interfacial dynamics with discontinuity is modeled by the continuous interface method (CIM), where the material properties and interfacial tension are smoothed out around interface by an approximate Dirac-delta function (δ_h)¹¹ within a four-cell width layer. This approach makes a single set of equations for all fluid phases in the entire domain. The approximate Dirac-delta function is used to transfer Lagrangian interfacial quantity to Eulerian fluid quantity, and vice

versa. The smoothed fluid properties across interface are computed by:

$$\phi = \phi_2 + (\phi_1 - \phi_2)I(\mathbf{x}), \quad (1)$$

where the subscript 1 and 2 indicate each phase material, and ϕ is the fluid properties. The indicator function (I) at a given location (\mathbf{x}) is a scalar function varying from zero to one smoothly across interface, and can be computed as a discrete form of the Heaviside step function (H) of approximate Dirac-delta function by:

$$I(\mathbf{x}) = H\left(r = \hat{\mathbf{n}} \cdot (\mathbf{x} - \mathbf{x}_f)\right) = \int_{-\infty}^r \int \delta_h(h) dh, \quad (2)$$

in which, $\hat{\mathbf{n}}$ is unit vector normal to interface, and subscript f means interface between different phases.

With the help of these approximate Dirac-delta function and indicator function, a single set of conservation equations for mass, momentum, and energy for the entire flow are written as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (3)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mu (\nabla \mathbf{u} + \nabla^T \mathbf{u}) + \mathbf{F}_f, \quad (4)$$

$$\frac{\partial \rho C_p T}{\partial t} + \nabla \cdot (\rho C_p T \mathbf{u}) = \nabla \cdot (k \nabla T). \quad (5)$$

Here, the vector \mathbf{u} is the velocity vector, and the material properties ρ , μ , C_p , and k are the density, viscosity, specific heat capacity, and thermal conductivity, respectively. In addition, t , p and T are time, pressure and temperature. The interfacial dynamics are accounted for by the momentum source (\mathbf{F}_f) from the phase boundary conditions.

In the normal direction, the phase boundary conditions accounting for the pressure (p) jump and stress tensor (τ) jump are related to the interfacial tension (σ) and the curvature (κ) of the interface by:

$$(p_2 - p_1) - \hat{\mathbf{n}} \cdot (\tau_2 - \tau_1) \cdot \hat{\mathbf{n}} = \sigma \kappa. \quad (6)$$

From this phase boundary condition, the normal component of the momentum source (\mathbf{F}_f) at a given location (\mathbf{x}) can be computed along phase boundary (Γ) directly by:

$$\mathbf{F}_{f,n}(\mathbf{x}) = \int_{\Gamma(t)} \left[\sigma (T_f(\mathbf{x})) \kappa(\mathbf{x}) \cdot \hat{\mathbf{n}} \right] \delta_h(\mathbf{x} - \mathbf{x}_f) d\Gamma. \quad (7)$$

The tangential component of the momentum source is incorporated into the Eulerian grids when there exists temperature gradient along the interface, given by:

$$\mathbf{F}_{f,t}(\mathbf{x}) = \int_{\Gamma(t)} \left[\nabla \sigma (T_f(\mathbf{x})) \cdot \hat{\mathbf{t}} \right] \delta_h(\mathbf{x} - \mathbf{x}_f) d\Gamma. \quad (8)$$

The interfacial tension typically decreases with temperature, and a piecewise linear approximation is used to compute accurate interfacial tension according to the temperature at each location along interface. The single set of conservation equations for mass, momentum, and energy for the entire flow in Eqs. (3)-(5) are solved using a projection method, where an intermediate velocity field is computed and projected into a divergence-free space. The convection term is discretized using the third-order ENO scheme in space and the second-order Runge–Kutta integration in time. The central difference scheme along with the Crank–Nicholson method is implemented for the viscous term. The pressure Poisson equation for the velocity correction is solved using the conjugate gradient method. The finite volume method is implemented with the staggered grid arrangement.

To effectively resolve the multiphase flow of multiple length and time scales, an adaptive mesh refinement (AMR) is implemented. The cells are split into four equal sibling cells. The grid is represented using unstructured data that connects cells through cell faces. The computational cells are dynamically refined based on the solution of the flow field and the movement of the micro-droplet. The details of the algorithm can be found in the previous study.^{9,10}

Results and Discussion

As a reference case, a micro-droplet with a diameter of $2 \mu\text{m}$ is simulated under temperature-gradients of 1000 K/mm . Figure 3 shows the streamlines of convective flow around a micro-droplet, where the shear flow and inner circulation are observed clearly. The temperature difference along the micro-droplet surface induces interfacial tension gradient, and the surface movement by interfacial tension creates outer shear flow and inner Marangoni convection.

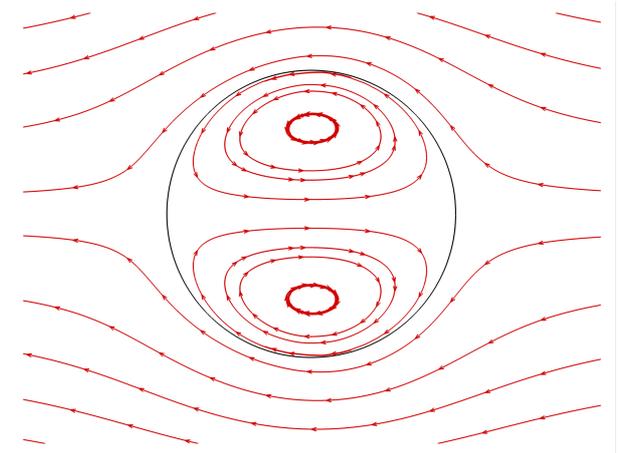


Figure 3. The streamlines around a micro-droplet in an emulsion droplet. The streamlines are plotted using the relative velocities to the micro-droplet to illustrate flow motions inside and around a micro-droplet separately.

In order to confirm the influence of the Marangoni effect and the mechanism of the micro-droplet movement, two different interfacial tension models are compared; the constant and temperature-dependent interfacial tension models. The diameter of a micro-droplet is $1\ \mu\text{m}$ and temperature gradient of $2000\ \text{K/mm}$ is assumed. The velocity-gradient of $500\ \text{s}^{-1}$ is applied on the computational domain based on our previous research on the droplet evaporation by local heating.¹⁰ This velocity gradient is identical to the velocity-difference of $10\ \text{cm/s}$ in $200\ \mu\text{m}$ between from the Hill's vortex center to the surface of emulsion droplet.

Figure 4 shows the x-directional movement of a micro-droplet in the given temperature- and velocity-gradients. In the unphysical constant interfacial tension model, the micro-droplet doesn't move to either of x-direction and it just moves along the Hill's vortex flow in y-direction. In the temperature-dependent interfacial tension model, the micro-droplet moves to cold region by shear flow in the initial transient period. However, the micro-droplet changes the direction and continues to move to hot surface after short transient time.

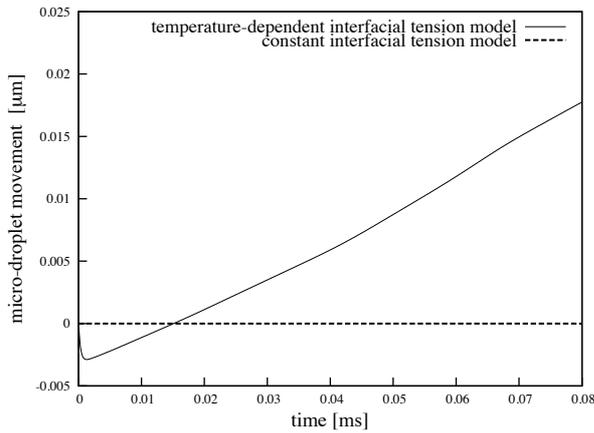


Figure 4. The comparison of the micro-droplet movements between constant and temperature-dependent interfacial tension models.

The difference of micro-droplet physics between two interfacial tension models is shown clearly in the micro-droplet velocity plot of Fig. 5. For the constant interfacial tension model, the x-directional velocity can be negligible. However, the micro-droplet moves to hot surface at $0.1\text{-}0.2\ \text{mm/s}$ for the temperature-dependent interfacial tension model. This results match well experiment by Chung and Kim³, where it takes several seconds until micro-droplets evaporate completely. The micro-droplet movement until emulsion droplet lifetime can be estimated as $0.3\ \text{mm}$, and this is enough to reach the evaporating surface of emulsion droplet and to vaporize first. From this comparison, it can be concluded that the interfacial tension difference by temperature gradient, namely Marangoni effect, is the key mechanism to transport micro-droplets to hot surface of an emulsion droplet.

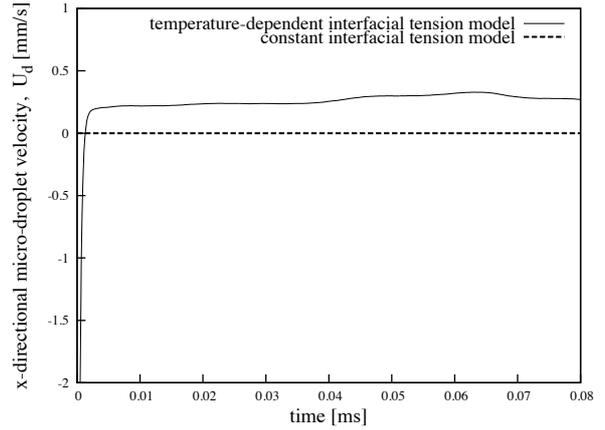


Figure 5. The comparison of the x-directional velocity of a micro-droplet between constant and temperature-dependent interfacial tension models.

The physics of micro-droplets in an emulsion droplet are compared between different types of emulsion droplets; water-in-oil and oil-in-water emulsion droplets. Figure 6 shows the velocities of micro-droplets with a diameter of $2\ \mu\text{m}$ under temperature gradient of $500\ \text{K/mm}$ for each type of emulsion droplet, where the oil micro-droplet moves faster in the oil-in-water emulsion droplet than water micro-droplet does in the water-in-oil emulsion droplet. The smaller density of oil can be one of the reasons for the phenomena. However, the normalized temperature difference plot in Fig. 7 clearly shows the major reason. The temperature difference of an oil micro-droplet surface increases in time unlike a water micro-droplet, and the larger temperature difference results in more Marangoni effect and faster velocities. The plot of temperature iso-contours in Fig. 8 explains that the difference of thermal conductivity causes temperature differences. For a given heat flux, larger thermal conductivity of water makes smaller temperature gradient inside a water micro-droplet, and following lower velocity by smaller Marangoni effect.

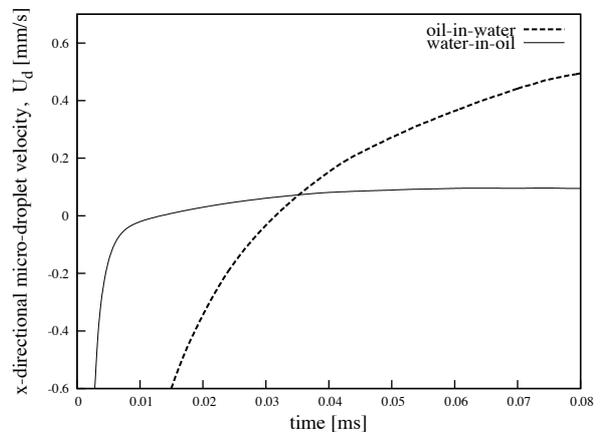


Figure 6. The comparison of micro-droplet velocities history in water-in-oil and oil-in-water emulsion droplets.

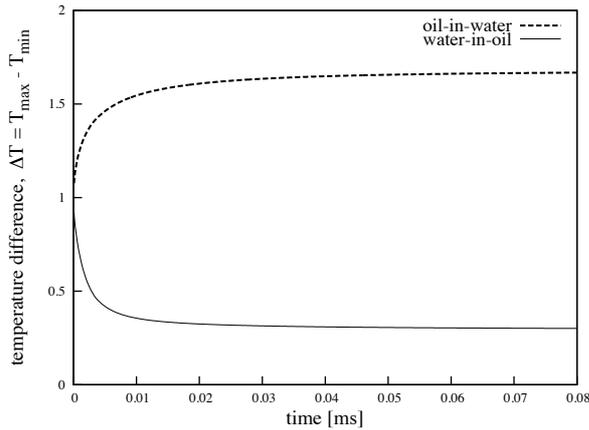


Figure 7. The comparison of the temperature difference in the micro-droplet surface for water-in-oil and oil-in-water emulsion droplets.

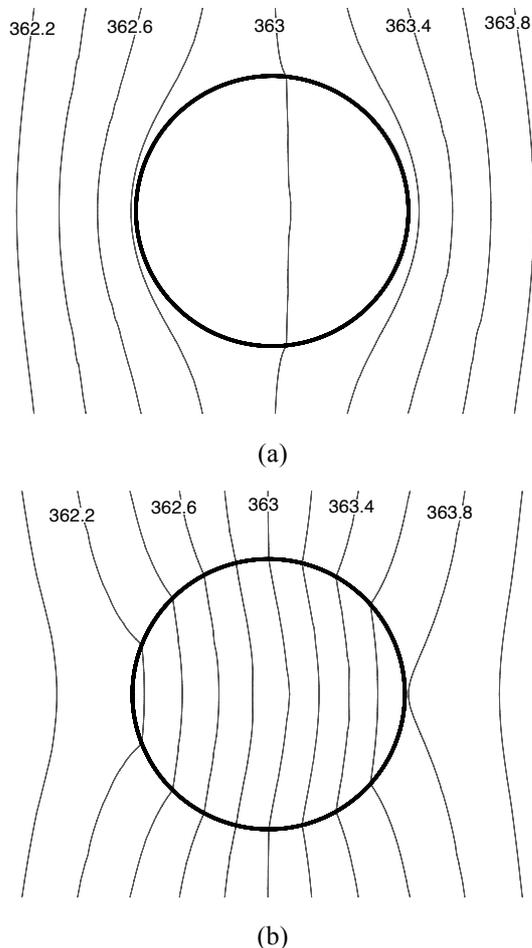


Figure 8. The comparison of temperature contours between different types of emulsion droplets; water-in-oil and oil-in-water emulsion droplets. (a) Water-in-oil emulsion droplet case; smaller temperature gradients due to large thermal conductivity of water. (b) Oil-in-water emulsion droplet case; large temperature gradient due to smaller thermal conductivity of oil.

Conclusions

In this study, the mechanism of the micro-droplet transportation to the hot surface of an emulsion droplet was investigated. The Eulerian-Lagrangian method was implemented with a temperature-dependent interfacial tension model for the computation of thermo-capillary interfacial dynamics of a micro-droplet. The comparison between constant and temperature-dependent interfacial tension model showed that the interfacial tension difference by the temperature gradient, namely the Marangoni effect, is the key mechanism to drive the micro-droplet to the higher temperature region. The comparison between water-in-oil and oil-in-water emulsion droplets confirmed that micro-droplets always move to hot surface for both types of emulsion droplets. Furthermore, it showed that the micro-droplet with larger thermal conductivity moves slower due to smaller temperature gradients inside a micro-droplet. This explains why oil micro-droplets in an oil-in-water emulsion droplet in general move faster.

Acknowledgments

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