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A computational study of droplet evaporation with fuel vapor jet ejection induced by localized heat sources

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Droplet evaporation by a localized heat source under microgravity conditions was numerically investigated in an attempt to understand the mechanism of the fuel vapor jet ejection, which was observed experimentally during the flame spread through a droplet array. An Eulerian-Lagrangian method was implemented with a temperature-dependent surface tension model and a local phase change model in order to effectively capture the interfacial dynamics between liquid droplet and surrounding air. It was found that the surface tension gradient caused by the temperature variation within the droplet creates a thermo-capillary effect, known as the Marangoni effect, creating an internal flow circulation and outer shear flow which drives the fuel vapor into a tail jet. A parametric study demonstrated that the Marangoni effect is indeed significant at realistic droplet combustion conditions, resulting in a higher evaporation constant. A modified Marangoni number was derived in order to represent the surface force characteristics. The results at different pressure conditions indicated that the nonmonotonic response of the evaporation rate to pressure may also be attributed to the Marangoni effect. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4919809>]

I. INTRODUCTION

The evaporation and combustion processes of liquid fuel droplets in a spray play a crucial role in the development of high efficiency and low emission engines. The combustion of a single droplet has been extensively studied, especially with a quasi-steady assumption,^{1–3} and at microgravity conditions in favor of the spherical symmetry for simpler analysis and interpretation.^{4,5} In practical combustion systems, however, flames spread through a spray cloud, and the physical process is much more complicated due to interactions between burning and unburned droplets. As such, direct application of the single droplet analysis to practical combustor simulations is likely to create large uncertainties in the prediction of the overall evaporation and burning characteristics.

Experimental studies have been conducted to characterize the flame propagation mechanism in the presence of fuel spray,^{6–8} in which different combustion modes were identified depending on the spray density. For a systematic investigation of the flame-spray interaction, flame spread along an array of droplets has been extensively investigated. One of the earlier studies by Reichenbach *et al.*⁹ reported a correlation between the flame propagation rates for various droplet sizes and spacing. Subsequent experimental studies^{10–12} conducted at normal and microgravity conditions found a maximum flame spread rate at an optimal droplet spacing. The influence of the ambient temperature has also been studied.^{13,14}

Another important parameter is the effect of pressure, for its practical relevance to engine combustion.¹⁵ At normal gravity conditions, Kato *et al.*¹¹ reported that the flame spread rate decreases monotonically with pressure until it ceases to propagate. Under microgravity conditions, Kobayashi *et al.*¹⁶ conducted experiment with an n-decane droplet array, up to 14 droplets with a diameter of 1.0 mm, in the supercritical pressure range up to 5.0 MPa. The results showed a

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FIG. 1. Computational approaches for the interface representation: (a) Lagrangian methods, (b) Eulerian (VOF) methods, and (c) Eulerian-Lagrangian methods.

nonmonotonic response in that the flame spread rate reaches a minimum value at about half the critical pressure, increases to a maximum value at above critical pressure, and then decreases again. In their study, a fuel vapor jet from the evaporating droplet was observed, which contributed to increasing the flame spread rate at near the critical pressure conditions by enhancing heat and mass transfer to the neighboring unburned droplet. A similar jet-like flow was also observed experimentally in the flame spread over an electrical wire.¹⁷ It was conjectured¹⁶ that the Marangoni effect induced by the temperature-dependent surface tension may be responsible for the fuel vapor jet ejection, but such a hypothesis has not been verified due to the lack of detailed information inside the droplets. The Marangoni effect on the vaporizing droplet in a high temperature convective flow fields has been investigated in the past.^{18–20} In these studies, however, the main interest was the change of the drag force due to the Marangoni effect in the presence of a strong convective flow. Furthermore, many simplifying assumptions employed in these studies, such as quasi-steadiness,¹⁸ quiescent liquid,¹⁹ or vorticity-stream function formulation,^{19,20} along with the existence of strong forced convective flow limit the understanding of thermo-capillary flow effect and the mechanism of vapor jet ejection.

Considering the difficulties in detailed experimental measurements, high-fidelity computational modeling is well suited to investigate the physical mechanism for these phenomena. For accurate prediction of relevant physical process, however, the computational method must be able to describe the multiphase interfacial dynamics with realistic surface tension and evaporation characteristics. Moreover, high-resolution grids are needed to capture the complex interfacial dynamics around the droplet surfaces. One of the most critical requirements is an accurate tracking of the interface location, since the calculation of the surface tension is directly related to the precise interface geometry. Among many existing computational methods,²¹ Eulerian methods such as the volume-of-fluid (VOF)²² and level-set²³ techniques have been commonly used in favor of their simplicity in numerical implementation. For both approaches, however, the accuracy of the interface representation is limited due to implicit tracking of the interface via a scalar function in a cell. The Lagrangian method with a body-fitted grid is most accurate for the present purpose, although maintaining satisfactory grid quality remains a challenge, especially when large deformation or topological changes take place.²⁴ As a rational compromise, the Eulerian-Lagrangian method (e.g., the immersed boundary method) utilizes a separate set of Lagrangian moving mesh associated with a marker/tag system representing the interface, which is overlaid on stationary Eulerian grids to compute the flow fields.²⁵ As such, the interface representation is achieved with high accuracy and does not require modifications to the computational grid of the field equations. Within some high order interpolation errors, the explicit tracking of the interface results in higher fidelity for the same level of grid resolution, in comparison with Eulerian methods at the same level of computational cost.²⁶ The principles of the three modeling approaches are illustrated in Figure 1.

For the modeling of the evaporation and mass transfer processes, accurate determination of the latent heat is essential in obtaining correct interfacial conditions. Juric and Tryggvason²⁷ treated the latent heat as a source term of energy equation implicitly using a Newton iteration technique

FIG. 2. The numerical configuration of the droplet evaporation simulation in the axisymmetric computational domain.

with the mass transfer rate treated as an unknown quantity. The method was simplified by Shin and Juric²⁸ with explicit mass transfer computation, while maintaining the diffused latent heat source term. Although this approach offers a simple solution, the accuracy degrades at higher phase change rate. Alternatively, Son and Dhir²⁹ solved a boiling bubble problem using the level set method by assuming the temperature inside the bubble to be constant without the latent heat source term. The homogeneous temperature assumption was commonly accepted for its simplicity and was adopted by Welch and Wilson.³⁰ Despite their successful implementations, none of these approaches are applicable to the present study because the uniform interface temperature assumption is only valid for droplet evaporation with spherical symmetry. In this study, however, it is critical to capture the interaction between the droplet heating and induced convective flow around the droplet, and thus the local droplet surface temperature must also be determined by proper physical conditions.

Therefore, the objective of the present study is to develop high fidelity models and reproduce the experimentally observed fuel vapor jet ejection process by simulations, in order to provide insights into the detailed physical mechanism for the phenomena. An Eulerian-Lagrangian method^{26,34} is modified for the interfacial dynamics computation by incorporating temperature-dependent surface tension model and a new local phase change model. An adaptive mesh refinement (AMR) is also employed in order to resolve the interfacial dynamics including surface tension and evaporation with high computational efficiency. The comparison of the representative simulations clearly demonstrates that the surface tension variation plays the key role in the observed phenomena. Subsequently, a parametric study is conducted by varying the droplet diameters and the temperature difference. A characteristic Marangoni number and time scale are proposed, with which the parametric results are correlated. Effects of the ambient pressure on the droplet evaporation are also investigated.

II. NUMERICAL METHOD

A. Problem configuration

A simplified model problem to represent flame-induced droplet evaporation and fuel vapor jet ejection is set up as shown in Figure 2. A liquid droplet of n-decane, as used in the Kobayashi's experiment,¹⁶ is heated by a high temperature source reasonably simulating a stationary flat flame at a constant temperature of 1500 K, which is imposed at the left boundary at the ambient pressure of 1.0 MPa, well below the critical pressure of 2.1 MPa. The initial droplet diameter (D_0) varies from 0.1 to 2.1 mm, and the distance between the droplet and the high temperature source is fixed at 0.5 mm for all droplet sizes considered. The computational domain size is taken sufficiently large to ensure that the solution field near the droplet is unaffected by the downstream and upper boundaries, at which zero temperature gradient and ambient pressure conditions are imposed. For computational efficiency, axisymmetry around the centerline is assumed.

A main objective of the study is to demonstrate that the surface-tension-driven flow along the droplet surface could generate the fuel vapor jet observed experimentally.¹⁶ To reproduce the

TABLE I. Material properties of n-decane (liquid) and air at 565.2 K at 1.0 MPa.³²

	n-decane (liquid)	Air
Density ρ (kg m ⁻³)	463.2	6.943
Density ratio (liquid to vapor) ρ_{lv}	10.29	
Viscosity μ (kg m ⁻¹ s ⁻¹)	8.548×10^{-5}	2.180×10^{-5}
Specific heat capacity C_P (J kg ⁻¹ K ⁻¹)	3.496×10^3	1.0342×10^3
Thermal conductivity k (W m ⁻¹ K ⁻¹)	0.075 80	0.0317
Surface tension σ (N m ⁻¹)	0.002 402 ($\sigma_T = d\sigma/dT = -6.136 \times 10^{-5}$)	

physical results with minimal computational cost, various simplifying assumptions are employed. At the reference pressure of 1.0 MPa, the initial temperature of the droplet and air is chosen at 560 K, close to the saturation temperature of n-decane (565.2 K) in order to avoid excessive grid resolution requirements. The pressure at 1.0 MPa was chosen because this falls into the range at which an increase in the flame spread rate was observed,¹⁶ hence is most susceptible to exhibit the Marangoni effect. In any case, a proper scaling relation will be obtained in terms of the Marangoni number. Furthermore, the choice is justifiable in the practical context considering that the spray droplets are expected to be heated up significantly before they interact with the flame. The center of droplet is fixed for all cases and the droplet deformation is neglected. As such, the distance between the heat source and the frontal droplet surface is kept constant in order to ensure the same level of heat flux from the local heat source.

The fuel evaporation processes are only considered without considering chemical reaction with the physical properties obtained from the NIST chemistry webbook³² as summarized in Table I. It is assumed that liquid fuel is evaporated when it reaches boiling point at a given pressure.

B. Multiphase modeling: Eulerian-Lagrangian method

Droplet evaporation by a localized heat source is essentially a multi-dimensional and unsteady process, such that typical 1D quasi-steady droplet evaporation models are not adequate. In this study, a marker-based Eulerian-Lagrangian method³¹ is implemented with a temperature-dependent surface tension model and a local phase change model to predict the thermo-capillary flow and the droplet evaporation rate. The method is chosen in favor of its accurate interface representation and explicit tracking. Capturing the interface geometry is crucial since it determines the accuracy of computing the surface tension and associated convective heat transfer.

The interfacial dynamics with discontinuity and surface tension between gas and liquid is modeled by the continuous interface method (CIM), where the material properties across interfaces are smoothed out by an approximate Dirac-delta function (δ_h) within a four-cell width layer,³³ such that a single set of equations for all fluid phases is solved in the entire domain. The approximate Dirac-delta function is also used to interpolate between the Lagrangian interfacial quantities and the Eulerian fluid quantities. The smoothed fluid properties across the interface are computed by

$$\varphi = \varphi_l + (\varphi_g - \varphi_l) I(\mathbf{x}), \quad (1)$$

where subscripts l and g indicate the liquid and gas phase, respectively, and φ is a fluid property such as the density (ρ), the ratio of density to viscosity (ρ/μ), and the inverse of thermal conductivity ($1/k$). The scalar indicator function (I) at a given location $\mathbf{x}(x, r)$ on the axisymmetric x - r plane varies smoothly from zero to one across the interface, having 0.5 at the interface location. For better accuracy near the boundary, this indicator function is computed as a discrete form of the Heaviside step-function (H) by

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

in which $\mathbf{n}$ is the unit vector normal to the interface, and the subscript f denotes the interface between the two phases.

Using the 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

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

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

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

where $\mathbf{u}(\mathbf{x}, t)$ is the velocity vector with the axial velocity component u and radial velocity component v in the axisymmetric x - r domain; t , p , and T are the time, pressure, and temperature, respectively.

The interfacial dynamics are accounted for by the momentum source ($\mathbf{F}_f$) and by the energy source (Q_f) from the phase boundary conditions. In the normal direction ($\mathbf{n}$), the phase boundary conditions accounting for the discontinuities in the mass, pressure, and heat are written as

$$\dot{m}_f = \rho_v (\mathbf{u}_f - \mathbf{u}_v) \cdot \mathbf{n} = \rho_l (\mathbf{u}_f - \mathbf{u}_l) \cdot \mathbf{n}, \quad (6)$$

$$(p_l - p_g) - \mathbf{n} \cdot (\boldsymbol{\tau}_l - \boldsymbol{\tau}_g) \cdot \mathbf{n} = \sigma \kappa, \quad (7)$$

$$(\mathbf{q}_g - \mathbf{q}_l) \cdot \mathbf{n} = \dot{m}_f h_{lv}, \quad (8)$$

where $\dot{m}_f$ is the mass transfer rate per unit interface area across the phase boundary and subscript v denotes the vapor phase. The jumps in pressure (p) and stress tensor ($\boldsymbol{\tau}$) across the phase boundary are related to the surface tension (σ) and the curvature (κ) of the interface. Similarly, the jump in the heat flux vector ($\mathbf{q}$) across the interface corresponds to the latent heat h_{lv} .

Continuity equation (3) can be completed by the phase boundary condition, Eq. (6). Without phase change phenomena such as evaporation, Eq. (3) is simplified to the divergence-free condition ($\nabla \cdot \mathbf{u} = 0$) to recover the incompressible flow formulation. In the presence of phase change, however, the divergence of the velocity is not zero and is computed by using the jump condition, Eq. (6), yielding

$$\nabla \cdot \mathbf{u} = (\mathbf{u}_v - \mathbf{u}_l) \cdot \mathbf{n} = \dot{m}_f \left(\frac{1}{\rho_v} - \frac{1}{\rho_l} \right). \quad (9)$$

To solve the momentum conservation equation, the momentum source by the surface tension must be obtained first. From Eq. (7), the normal component of the momentum source ($\mathbf{F}_f$) at a given location ($\mathbf{x}$) can be computed along the phase boundary (Γ) by

$$\mathbf{F}_f \cdot \mathbf{n} = \int_{\Gamma(t)} [\sigma(T_f(\mathbf{x})) \kappa(\mathbf{x}) \cdot \mathbf{n}] \delta_h(\mathbf{x} - \mathbf{x}_f) d\Gamma. \quad (10)$$

The tangential component of the momentum source ($\mathbf{F}_f$) is incorporated with the unit vector tangential to interface ($\mathbf{t}$) into the Eulerian grids when there exists temperature gradient along the interface given by

$$\mathbf{F}_f \cdot \mathbf{t} = \int_{\Gamma(t)} \left[\frac{d\sigma(T_f(\mathbf{x}))}{d(\mathbf{x} \cdot \mathbf{t})} \cdot \mathbf{t} \right] \delta_h(\mathbf{x} - \mathbf{x}_f) d\Gamma. \quad (11)$$

Surface tension typically decreases with temperature. A piecewise linear approximation is used to compute accurate surface tension according to the temperature at each location along the interface. The surface tension force on a discretized interface can be directly computed by the curvature using the surface fitting. However, interpolation-based curvature computation is sensitive to data-smoothing and does not guarantee the conservation of the net surface tension for the entire droplet. Therefore, the line integral form is computed in the normal and tangential directions of the interface elements. This approach is much easier to implement and ensures the conservation properties without expensive curvature computation.²⁵

During the evaporation process, the liquid is transformed to the vapor, and the difference of enthalpy is used for the evaporation energy. The critical modeling issues are (1) how to compute the

amount of the mass transfer and (2) how to treat the latent heat, because they are directly related to the vapor concentration, phase boundary movement, and the resulting temperature distribution.

As the local interface temperature reaches the boiling temperature, the mass transfer across the interface is computed from the interfacial boundary condition based on the Stefan condition given by

$$\dot{m}_f h_{lv} = (\mathbf{q}_g - \mathbf{q}_l) \cdot \mathbf{n} = -k_g \left. \frac{\partial T}{\partial n} \right|_g + k_l \left. \frac{\partial T}{\partial n} \right|_l, \quad (12)$$

where the difference in heat flux $\mathbf{q}$ is determined by the temperature gradient in each phase. The local interface temperature at each node of the interface mesh is interpolated from the neighboring cells using AMR for improved accuracy. The thermal conductivity of each phase, k_g and k_l , is utilized for accurate mass transfer computation even though the overall energy equation is solved with smoothed material properties via the aforementioned continuous interface method.

Once the mass transfer rate per unit interface area ($\dot{m}_f$) is determined, the latent heat resulted from evaporation is determined for the energy conservation equation. Similar to the momentum source, the energy source (Q_f) in Eq. (5) in the Eulerian form is computed from the Lagrangian equation via the approximate Dirac-delta function by

$$Q_f = \int_{\Gamma(t)} \dot{m}_f h_{lv} \delta_h(\mathbf{x} - \mathbf{x}_f) d\Gamma. \quad (13)$$

While the amount of fuel evaporation and vapor production is accurately determined by the correct thermodynamic properties and the ratio of liquid density to fuel vapor density (ρ_{lv}), the evaporated fuel vapor is passively advected by the surrounding flow field. Near the surface of a fuel droplet, the velocity field is dominated by the surface tension and the mass diffusion is negligible compared to the convective transport. Far from the droplet and vapor jet flow, the fuel vapor concentration is sufficiently small and has little effect on the quantitative result. Based on this consideration, the multi-species gas-phase solutions are described as a single-species gas flow with the additional information of fuel vapor concentration ϕ , which is computed only for the gas phase from the simple advection equation by

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = \frac{2}{\rho_v} \int_{\Gamma(t)} \dot{m}_f \delta_h(\mathbf{x} - \mathbf{x}_f) d\Gamma, \quad (14)$$

where the RHS term represents the change of the vapor volume by evaporation of the liquid fuel, for which zero normal-velocity boundary condition is applied on the droplet surface.

Only one set of the governing equations including energy equation is solved throughout the entire domain using the continuous interface method. The phase change occurs only when the local interface temperature reaches the boiling temperature. The local interface temperature is interpolated from the temperature of neighboring cells, and additional resolution was implemented by an AMR in the region of steep changes in the temperature gradient across interface. For simplicity, the boiling temperature is assumed to be equal to the saturation temperature at a given ambient pressure. For the implementation of latent heat and evaporation, the mass transfer is computed locally where the interface temperature reaches the boiling temperature.

The interfaces between the liquid and gas phases are represented and tracked by moving Lagrangian meshes, which are established by line segments in the spherical axisymmetric computation. The Lagrangian meshes move relative to the Eulerian grid at the local velocities determined by

$$\frac{\partial \mathbf{x}_f}{\partial t} = \mathbf{u}_f(\mathbf{x}_f) = \mathbf{V}_{fl} + \mathbf{V}_{pc}, \quad (15)$$

where $\mathbf{x}_f$ is the interface location vector, determined by the fluid velocity, $\mathbf{V}_{fl}$, and the surface velocity due to the phase change, $\mathbf{V}_{pc} = \dot{m}_f / \rho_l$. This continuous interface method can be effective in highly deformable and moving droplet surfaces.

A single set of conservation equations for the entire flow domain is solved using a projection method, where an intermediate velocity field is computed and projected onto a divergence-free space. The convection term is discretized using a third-order essentially non-oscillatory (ENO)

FIG. 3. An example of adaptive mesh refinement. Different adaptation level and layers are implemented for the appropriate grid resolution. Highest resolution is applied around the droplet surface for accurate interfacial dynamics computation. Adaptation is implemented dynamically based on the solution in time.

scheme in space and a second-order Runge–Kutta integration in time, and the viscous term is discretized by a central difference scheme along with the Crank–Nicholson method. The pressure Poisson equation for the velocity correction step is solved using a conjugate gradient method. The finite volume formulation is implemented with the staggered grid arrangement.

C. Adaptive mesh refinement

Multiphase flow involves multiple length and time scales. In particular, in the phase change problem with steep changes in temperature gradients, the resolution around the interface is important in accurate prediction of the mass transfer rate. To effectively resolve the flow features in such cases, an AMR is implemented. The cells are split into four equal sibling cells, and the grid is represented using unstructured data that connect cells through cell faces. The details of the algorithm can be found in the previous study.³¹

The adaptive algorithm is further refined by implementing different AMR levels and layers for each region. Figure 3 shows an example of the AMR in the present simulation. For a geometry-based adaptation, a maximum of seven refinement levels is used with six adaptation layers around the droplet surface where the grid refinement is needed most. Along the boundaries of the high temperature source and axisymmetry, a moderate level of four refinements is used with a relatively lower four-layer adaptation. Similarly, solution-based adaptation based on the vapor concentration and flow features is made also with four-level refinement. Relatively lower solution-based adaptation criteria are used because the finest grid resolution is required along the interface in this droplet evaporation problem. Furthermore, the computational cells are dynamically refined based on the solution of the flow field and the droplet deformation along with evaporation.

III. RESULTS AND DISCUSSION

A. Mechanism of fuel vapor jet ejection

As a reference case, an *n*-decane droplet with the initial diameter (D_0) of 1 mm is simulated under zero-gravity and ambient pressure (P_0) of 1.0 MPa. The surrounding air is initially quiescent. The initial temperature (T_0) for the droplet and surrounding air was set at 560 K. The vertical heat source of 1500 K was located on the left side by 0.5 mm from the droplet.

Figure 4 shows the temporal evolution of the droplet surface temperature distribution along the droplet surface, which is rapidly heated to the boiling temperature. The temperature gradient is large in the beginning and subsequently decreases with time. At $t = 0.1$ s, the temperature becomes uniform along the entire surface of the droplet and reaches the boiling temperature.

Until $t = 0.10$ s, the temperature gradient induces a surface tension gradient and consequently drives the internal flow motion. The surface tension decreases on the hotter surface region (left side)

FIG. 4. The evolution of the droplet surface temperature. Distance along droplet surface (l) is the distance measured from the hot stagnation point near heat source along the droplet surface as defined in Figure 2.

as temperature increases by heat conduction, and the fluid element near droplet surface starts to move from a hotter to colder region because gradients in the surface tension cause surface traction forces away from the hotter spot. These surface movements cause the inner flow circulation, namely, the Marangoni convection, and outer shear flow around the droplet surface. The streamlines of the shear flow around the droplet and inner circulation and the color-coded u -velocity component in Figure 5 clearly show the developed flow motion. The mechanisms of the Marangoni effect and the induced convective flows are illustrated in Figure 6. The temperature difference by a local droplet heating creates surface tension gradients along the droplet surface and induces outer shear flow and inner Marangoni convection. The evaporated fuel vapor is then transported to the colder region (right side) by the outer shear flow, and such behavior is clearly reproduced in Figure 5.

To confirm the mechanism of the fuel vapor jet, a simplified constant surface tension model was simulated for comparison. Figure 7 shows the axial-directional u -velocity (upper) and temperature (lower) isocontours for the two models. In the constant surface tension model (a), the flow field is stationary because the Stefan flow by evaporation is the only flow motion near droplet and is much smaller than convective flow of Figure 7(b). Thus, the heat is transferred from the heat source to

FIG. 5. Streamlines and the axial-directional u -velocity isocontours (in color) to visualize the shear flow around the droplet and inner Marangoni convection.

FIG. 6. A schematic illustration of the Marangoni effect and the fuel vapor jet ejection mechanism.

the droplet only by the conduction. In contrast, the temperature-dependent surface tension model (b) predicts the development of the Marangoni convection inside the droplet and strong outer shear flow around the droplet. The temperature isocontours show that the heat is transferred to the cold region along the droplet surface by the induced strong outer shear flow. The Marangoni effect is largest in the beginning when the temperature gradient is the largest and gradually decreases as the surface temperature becomes uniform along the droplet surface.

Figure 8 shows the comparison of fuel vapor concentration between the two models. In the constant surface tension model, Figure 8(a), the fuel vapor is nearly quiescent on the high temperature source side due to the lack of the induced shear flow. In contrast, the temperature-dependent surface tension model, Figure 8(b), yields a significant fuel vapor jet ejection, because the induced outer shear flow by the Marangoni effect transports the fuel vapor along the droplet surface towards the wake region, forming a vapor jet. The results qualitatively reproduces the fuel vapor jet ejection observed in the experiment,¹⁶ thus confirms the original hypothesis of the study that the surface tension variation is the main cause. In spray combustion, such fuel vapor jets may promote heat and mass transfer to the neighboring unburned droplets and may contribute to the overall acceleration of the flame spreads rate in the intermediate pressure range, as observed by the experiment.¹⁶

B. Parametric study on the Marangoni effect

To characterize the Marangoni effect on the local droplet heating problems, a nondimensional number is introduced from a scaling analysis and a parametric study is conducted. The Marangoni effect is proportional to the temperature derivative of the surface tension ($\sigma_T = d\sigma/dT$) and the temperature gradient along the droplet surface (dT/dl), which is approximated by the ratio of the maximum temperature difference (ΔT) between the boiling temperature (T_b) and the initial droplet

FIG. 7. The axial-directional u -velocity and temperature isocontours for (a) constant and (b) temperature-dependent surface tension models.

FIG. 8. The comparisons of the fuel vapor jet ejections between the (a) constant and (b) temperature-dependent surface tension models.

temperature (T_0) to the half of the initial droplet perimeter ($\pi D_0/2$). The magnitude of the effect is proportional to the initial droplet surface area (A_0). Therefore, the net effect is described by a characteristic Marangoni number defined as

$$Ma = -\frac{\sigma_T \Delta T A_0}{\pi D_0 \mu_l \alpha_l}, \quad (16)$$

where α is the thermal diffusivity and subscripts 0 and l indicate the initial condition and the liquid phase of the droplet, respectively. The Marangoni number represents the ratio of surface tension to viscous forces. In the cylindrical case ($A_0 = \pi D_0$), Eq. (16) becomes $Ma = -\sigma_T \Delta T / (\mu_l \alpha_l)$ regardless of the droplet diameter. In the spherical axisymmetric case ($A_0 = \pi D_0^2$) considered in the present study, $Ma = -\sigma_T D_0 \Delta T / (\mu_l \alpha_l)$ degenerates to the identical form as that used in the well-known Benard-Marangoni convection,^{34,35} despite the fundamental differences between the two phenomena in terms of surface curvature and definitions of heat transfer and temperature difference.

To validate that Eq. (16) serves as a proper parameter characterizing the driving force, the actual surface tension force (F_s) is measured on the entire surface of a droplet during each case of simulations, and the normalized surface tension force is defined as

$$F_s^* = \frac{F_s}{\mu_l \alpha_l}. \quad (17)$$

Figure 9 shows the results compiled for the droplet diameter ranging from 0.05 mm to 2.0 mm and four different initial droplet temperature ($T_0 = 560, 561.3, 562.6$, and 563.9 K) values. The nondimensional surface force scales almost linearly with the Marangoni number for most cases except

FIG. 9. Maximum nondimensional surface force as a function of the Marangoni number.

in the region of very small Marangoni numbers. The deviation in the small Marangoni number conditions will be discussed later.

To further identify the characteristic time scales for the process, the Marangoni time scale is defined as follows. For a given Marangoni surface force ($F_M = -\sigma_T D_0 \Delta T$), the acceleration (a_M) of the droplet surface can be estimated by dividing the force by the droplet mass, such that

$$a_M \sim \frac{-\sigma_T \Delta T}{\pi \rho_l D_0^2}. \quad (18)$$

The time duration of the liquid and vapor movement, from the hot to cold stagnation point with a distance of $\pi D_0/2$, is then approximated by $(\pi D_0/a_M)^{1/2}$, which yields the characteristic Marangoni time scale as

$$t_M = \frac{\pi D_0^{3/2}}{(-\sigma_T \Delta T / \rho_l)^{1/2}}. \quad (19)$$

FIG. 10. The ratio of the nondimensional surface force to the Marangoni number as a function of the nondimensional time scale $(t - t_0)/t_M$.

FIG. 11. Maximum nondimensional surface force as a function of the effective Marangoni number defined by effective temperature difference.

Figure 10 shows the temporal evolution of the ratio of the nondimensional surface force to the Marangoni number as a function of the nondimensional time $(t-t_0)/t_M$, where the time axis is translated by t_0 , a case-dependent transient time related to the heat transfer from the hot temperature source to the droplet. For droplets with a diameter larger than 0.5 mm, a successful collapse of the curves for different cases is evident. The curves deviating from the collapsed curve, denoted as *under-developed* cases, correspond to the smaller droplets with (or without) larger temperature differences. In these cases, the smaller Marangoni time scale promotes a rapid heat transfer to the cold rear stagnation point along the droplet surface before the hot stagnation point reaches the boiling temperature. Therefore, the actual temperature difference between the front and back of the droplet surface is smaller than the given temperature difference ($\Delta T = T_b - T_0$). The smaller temperature difference results in reduced surface force due to the under-developed Marangoni effect, even at the same Marangoni number. Figure 11 shows these effects clearly. If the temperature difference is determined by $\Delta T = T_b - T_0$, denoted by solid triangles, the data points deviate from the straight line at smaller values of the Marangoni number.

FIG. 12. D^2 -law comparisons between a constant surface tension model and a temperature-dependent surface tension model.

FIG. 13. Maximum evaporation constant normalized by the ideal evaporation constant, $K_{ref} = (8k_g / (\rho_l C_{pg})) [\ln(1 + C_{pg}(T_\infty - T_b)/h_{lv})]$ as a function of the Marangoni number.

To compensate for the under-developed conditions, the Marangoni number may be determined with the *effective* temperature difference ($\Delta T_{eff} = T_{f,max} - T_{f,min}$). The results, denoted by the open squares, show a nearly linear scaling for all data points. The results confirm that the Marangoni effect is indeed the driving mechanism for the induced surface force.

C. Enhanced droplet evaporation rate

The temporal droplet evaporation behavior in the presence of the local droplet heating is subsequently compared with the ideal D^2 -law,^{2,3} based on the spherically symmetric configuration, which dictates that the square of droplet diameter decreases linearly with time. Figure 12 shows D^2 versus time for the constant and temperature-dependent surface tension models. The corresponding D^2 -law lines are overlaid in order to compare the slope, neglecting the initial droplets heating period. It is clearly shown that the temperature-dependent surface tension case shows the evaporation rate significantly higher than the slope predicted by the D^2 -law, confirming that the Marangoni effect has a net enhancement in the overall droplet evaporation rate.

Figure 13 further shows the compiled data for the maximum evaporation rate constant determined from the time derivative of the diameter of dD^2/dt , normalized by the ideal evaporation constant $K_{ref} = (8k_g / (\rho_l C_{pg})) [\ln(1 + C_{pg}(T_\infty - T_b)/h_{lv})]$, as a function of the Marangoni number. The results clearly indicate that the droplet evaporation rate increases with the Marangoni number. For a given Marangoni number, the effect is larger as the droplet size is increased, which is attributed to the thermal conduction inside the liquid droplet for small droplets.

Despite the successful simulations of the fuel vapor jet ejection shown in Figure 8, however, the magnitude of the vapor jet observed in the simulation is found to be smaller than the values in the experiment,¹⁶ where the jet velocity was estimated to be approximately 0.3 m/s based on the back-lit images. This is attributed to the differences in the simulation condition, in which the

TABLE II. Enthalpy of n-decane at initial and boiling temperature.³²

Ambient pressure P_0 (MPa)	Boiling temperature T_b (K)	Latent heat h_{lv} (J/kg)	$\Delta h = h(T_{b,v}) - h(T_0)$ (J/kg)
1.0	565.2	171 150	189 050
1.2	577.5	152 810	216 900
1.4	588.2	133 600	234 600

FIG. 14. The normalized droplet volume as a function of time at different pressure conditions.

pressure was set at 1.0 MPa, much lower than the experimental conditions of 3.0 MPa at which a strong jet flow was observed. Furthermore, the approaching flame in the experiment may enhance the Marangoni effect unlike the fixed high temperature source in this study. While it is difficult to simulate near-critical conditions due to the uncertainties in thermodynamic properties, an attempt is made to observe a general trend as the system pressure is increased.

As pressure increases, the latent heat for the n-decane droplet decreases as shown in Table II, implying that the droplet can be vaporized more easily. On the other hand, the boiling point increases such that it takes longer to heat up the droplet to the boiling temperature. These competing effects modify the overall droplet evaporation rate behavior at different pressures, and the enthalpy difference (Δh) from the same initial condition to evaporated vapor implies that more heat transfer is required for evaporation as ambient pressure increases.

Figure 14 shows the variation of droplet volume V normalized by the initial volume V_0 as a function of time at three different pressure conditions. At a higher ambient pressure, the droplet initially evaporates more slowly because the droplet must be heated to the higher boiling temperature. However, once the surface temperature of the droplet reaches the boiling temperature (T_b), the evaporation process increases more rapidly due to lower latent heat (h_{lv}) and stronger Marangoni effect induced by larger temperature difference between the initial droplet temperature and the boiling temperature. This indicates that the evaporation rate is enhanced at higher pressure due mainly to the increased Marangoni effect, although more heat transfer is required as shown in Table II. The results also support the experimental observation¹⁶ that the flame spread rate increases with pressure, from half of the critical pressure up to nearly the critical pressure condition.

IV. CONCLUSIONS

The droplet evaporation by a localized heat source was simulated in order to explain the mechanism of the fuel vapor jet ejection observed experimentally at micro-gravity conditions.¹⁶ It was found that the temperature difference by a local droplet heating induces the corresponding surface tension gradient along the droplet surface, developing a shear flow around the droplet and strong internal Marangoni convection. The induced shear flow subsequently leads to a fuel vapor jet ejection by driving the evaporated fuel to the wake region of the droplet. The comparison with a constant surface tension model confirmed that the mechanism of fuel vapor jet ejection was induced by the surface tension gradient resulting from the local heating. A characteristic Marangoni number and nondimensional time scale were derived and the results were found to collapse well in terms of the nondimensional parameters. It was shown that the surface force is proportional to the Marangoni number when the effect is fully developed, which happens for a larger droplet size and/or smaller

temperature difference. The strength of inner Marangoni convection was found to be proportional to $1/D_0^2$ as expected from scaling analysis. For the evaporation phenomena, the evaporation constant was similar to the ideal D^2 -law for constant surface tension model. With temperature-dependent surface tension model, however, the evaporation constant increases with the Marangoni number by due to the increased internal convection. It was also found that the evaporation rate is enhanced with increasing the ambient pressure due to increased heat transfer associated with the Marangoni effect, consistent with experimental observations.

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