

Interface-capturing numerical studies of multicomponent spray and droplet vaporization

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Motivated by improving theoretical understanding of spray combustion, this work studies the vaporization of multicomponent spray and droplets. The work performs an exploratory study of spray vaporization, however, focuses on the physics of droplet vaporization. For real fuels, which consist of multiple chemical species (or components), the combustion properties of the fuel will change in time depending of which components of the fuel are most represented in the vapor. This composition dependence is dominated by differences in the vaporization rates of the components. While much is known about the vaporization of fuel droplets, these studies have often used numerous simplifying assumptions. Recent work has begun to demonstrate that some of these neglected phenomena such as droplet deformation and internal liquid flow have appreciable effects on the vaporization of fuel droplets.

This work investigates how droplet deformation and internal flow affect the vaporization of a Jet-A surrogate. The work leverages an in-house finite volume code for performing interface-capturing direct numerical simulations of liquid-gas flows. The code simulates the dynamics of multicomponent-fuel vaporization from first principles by directly solving the governing conservation laws for mass, momentum, and energy transport. Results quantify how vaporization is affected by these phenomena in terms of appropriate non-dimensional groups such as the Weber number and the circulation strength and trends are discussed.

I. Some Nomenclature

ρ	=	Fluid density ($kg\ m^{-3}$)
μ	=	Fluid viscosity (a)
c_p	=	Specific heat ($J\ kg^{-1}\ K^{-1}$)
σ	=	Surface tension ($N\ m^{-1}$)
h_v	=	Latent heat of vaporization (enthalpy of vaporization) ($J\ kg^{-1}$)
M	=	Molar mass ($kg\ mol^{-1}$)
T_b	=	Boiling temperature (K)
D	=	Diffusivity ($m^2\ s^{-1}$)
λ	=	Thermal diffusivity ($m^2\ s^{-1}$)

II. Introduction

This work is motivated to better understand combustion as it occurs in aviation gas-turbine engines. In gas-turbine engines, a liquid fuel is injected into the combustor where it atomizes into droplets, the droplets vaporize, and the fuel vapor combusts. Understanding the vaporization is important since it determines the composition of chemical species in the gas phase that are available for combustion. This phenomenon is especially important for fuels that consist of multiple chemical species (or components) as the components may have different thermochemical properties resulting in different combustion behaviors. This is true of most common aviation fuels including Jet-A and JP-8, and therefore knowledge of multicomponent fuel vaporization is important to predicting the combustion of these fuels.

Traditionally spray have been simulated using a multifidelity strategy. Gas phase dynamics are solved using high-fidelity

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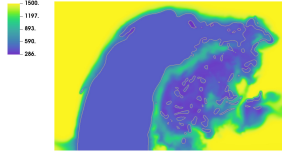


Fig. 1 Snapshot of temperature for simulation in Section IV. The gray contour is the liquid-gas interface.

strategies such as large eddy simulation or direct numerical simulation. However, liquid phase dynamics are represented as discrete droplets that obey Lagrangian equations of motion. This representation is unable to fully capture many phenomena relevant for multiphase simulations such as spray atomization, secondary atomization, and liquid internal mixing. Accordingly, they cannot capture their interaction with preferential vaporization of high volatility fuel components.

Only recently have strategies for true direct numerical simulation of vaporizing spray become possible [1, 2]. In this sense, a study is a true direct numerical simulation if it correctly captures liquid interface topology changes such as break-up as well as phase change phenomena. An example is demonstrated in Fig. 1 which demonstrates the temperature from the case in Section IV. In theory, such studies can yield a wealth of new information about spray. However, these studies are limited by their computational cost. They require meshes fine enough to resolve the smallest flow droplets, which may be an order of 1000 times smaller than the jet diameter. While, such strategies may become powerful tools for the investigation of low Reynolds number jets in the near future, they still cannot be used as a complete replacement for Lagrangian methods at this time.

The goal of this study is to demonstrate the capabilities of interface-capturing simulations as a tool for droplet analysis. The long term goal of this work will be to use these simulations to create databases of droplet vaporization, and these can eventually be used to develop next generation Lagrangian models. However, the development of such databases and models is not performed in this paper.

Vaporization of fuel droplets has been studied extensively in the literature from analytical, computational, and experimental perspectives [3–6]. However since interface-capturing simulation strategies have only been developed recently, many classical studies neglect physical process that are relevant for spray combustion. Vaporization has been typically been viewed as a gas phase heat and mass transfer problem, and the influence of two phase flow physics have traditionally been ignored. However recent results have shown that effects such as shear-induced internal droplet flow and the deformation of the droplets into non-spherical shapes have important effects on the vaporization of single component droplets [7–9]. The effects of these phenomena on multicomponent droplets should be explored. This study will seek to explore these effects through identification of the governing non-dimensional groups and the study thereof.

III. Methods

The work uses an in-house code for interface-capturing direct numerical simulations of liquid-gas flows with phase change. The framework is based largely on [2] which introduced a first principles based approach for studying the vaporization of single component fuels. The current work modifies that strategy to account for multicomponent fuels, and uses the updated work to study the preferential vaporization of a Jet-A surrogate [10]. The surrogate uses a mixture of 42.67/33.02/24.31 (by moles) of n-decane, iso-octane, and toluene.

A. Thermodynamic Strategy

The flow is considered to consist of two immiscible fluid phases, a liquid and a gas respectively. The phases are demarcated by a sharp interface of infinite thinness, so a separate transport equation must be introduced to represent the evolution of the interface. Each phase consists of several constituent chemical species (or components) that are miscible within that phase. The composition of each phase is represented by knowledge of the mass fractions of each component.

The code is adapted from an incompressible code for multiphase flows, so the following decomposition is used. Transport equations are computed using a constant property assumption. That is, they are computed without using information about the local fluid composition. This choice is considered for ease of implementation into the incompressible flow

solver, however, it will be re-investigated in the future. Such an approach will not work for resolution of preferential vaporization physics. It is precisely the difference in fluid properties which mediate preferential vaporization. Therefore the vaporization sources were computed using local information about the fluid composition. Vapor pressure was computed component-by-component using the Clausius-Clapeyron relation and Raoult's law, which in turn yield information about the composition of fuel vapors in the gas phase. And the latent heat at each location on the interface is computed using the resulting local information about the chemical composition.

B. Numerical Strategy

The work leverages a finite volume code for simulation of vaporizing liquid-gas flows that has been developed over the last few years [2, 11, 12]. The code is a true direct numerical simulation code since the evolution of all phenomena is solved via first principles.

All dynamics of the flow are derived from the transport equations. The liquid-gas interface is captured implicitly through the use of a geometric volume of fluid method [13]. The method tracks the local fraction of liquid volume in the computational cell (α) and uses this information to reconstruct the interface location and all relevant geometrical information like the interface normal vector, and the curvature κ [14, 15]. By convention, the curvature is considered positive when the liquid is locally convex.

Momentum solution occurs using a so-called one field approach where an effective density and viscosity are computed as

$$\rho = \rho_L \alpha + \rho_G (1 - \alpha), \quad (1)$$

$$\mu = \mu_L \alpha + \mu_G (1 - \alpha), \quad (2)$$

respectively. The subscripts L and G represent liquid and gas phase values of the quantity, respectively. The Navier-Stokes equations are then written as,

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot (\mu \mathbf{S}) + \mathbf{f} \quad (3a)$$

$$\mathbf{S} = \left(\nabla \mathbf{u} + \nabla \mathbf{u}^\top - \frac{2}{3} \nabla \cdot \mathbf{u} \right). \quad (3b)$$

Where the pressure is chosen to impose the continuity equation, and is solved via a pressure Poisson equation [2].

Vaporization causes the imposition of a Stefan flow which is the flow of vapor from the interface. From the mass conservation principle it can be shown,

$$[\mathbf{n} \cdot \mathbf{u}]_\Gamma = \dot{m} \left[\frac{1}{\rho} \right]_\Gamma \quad (4)$$

Here $\dot{m}$ is the vaporization rate (per unit area) and the bracket notation reflects $[\phi]_\Gamma = \phi_G - \phi_L$ for arbitrary field, ϕ . From the momentum equation it follows,

$$[p]_\Gamma = -\sigma \kappa - \dot{m}^2 \left[\frac{1}{\rho} \right]_\Gamma \quad (5)$$

where σ is the surface tension coefficient.

Scalars (chemical species and temperature) are treated sharply to ensure higher accuracy [16]. Under the assumption of a low Mach number flow, it is appropriate to write the energy equation in the liquid as,

$$\frac{\partial (\rho_L h_L)}{\partial t} + \nabla \cdot (\rho_L h_L \mathbf{u}) = \nabla \cdot (k_L \nabla T), \quad (6)$$

where k is the thermal conductivity. Using the definition of specific heat, $c_p = dh/dT$, this can be rewritten as

$$\frac{\partial (\rho_L c_{p,L} T_L)}{\partial t} + \nabla \cdot (\rho_L c_{p,L} T_L \mathbf{u}) = \nabla \cdot (\rho_L c_{p,L} \lambda_L \nabla T_L), \quad (7)$$

where $\lambda = k/(\rho c_p)$ is the thermal diffusivity. For a multicomponent liquid fuel, the composition of components within the liquid must also be described. The composition is quantified with the mass fractions. For an arbitrary species in the liquid, $Y_{L,x}$,

$$\frac{\partial (\rho_L Y_{L,x})}{\partial t} + \nabla \cdot (\rho_L Y_{L,x} \mathbf{u}) = \nabla \cdot (\rho_L D_{L,x} \nabla Y_{L,x}), \quad (8)$$

Similar equations can be written for the gas temperature and mass fractions. An important thing to note is that special algorithms are needed for computing the scalar advection and diffusion for grid cells near the interface. The approach used in this work follows the philosophy of finite volumes and computes these terms additional terms as fluxes integrated over the interface. Detailed description of the algorithms are listed elsewhere [2].

Although scalar are solved separately for each phase, the components are explicitly coupled through thermodynamic equilibrium at the interface. Although the mass fractions, Y_x , are convenient to describe the composition for transport, the mole fractions, χ_x , are more convenient for describing thermodynamic equilibrium. These quantities are easily converted via their definitions,

$$\chi_k = \frac{Y_k}{W_k} \left(\sum_x \frac{Y_x}{W_x} \right)^{-1} \quad (9)$$

$$Y_k = W_k \chi_k \left(\sum_x W_x \chi_x \right)^{-1} \quad (10)$$

where the molar mass of the species, W_x , is introduced.

For multicomponent mixtures, the relevant law of thermodynamic equilibrium is Raoult's law,

$$\chi_{G,x} = \chi_{L,x} \chi_{G,x}^* \quad (11)$$

which expresses a relationship between the actual vapor mole fraction ($\chi_{G,x}$) of a species in the gas, the equilibrium vapor fraction ($\chi_{G,x}^*$) of that species, and the mole fraction of that species in the liquid, $\chi_{L,x}$. $\chi_{G,x}^*$ can be computed from the phase equilibrium curve of the fluid $_x$. For an ideal gas, this can be computed using the Clausius-Clapeyron relation,

$$\chi_{G,x}^* = \exp \left[-\frac{h_{v,x} W_x}{R^\circ} \left(\frac{1}{T} - \frac{1}{T_{b,x}} \right) \right] \quad (12)$$

where the universal gas constant, R° and the boiling temperature of the species $T_{b,x}$ are introduced.

These equations couple the specification of the interface vapor conditions with the temperature. However, the system is also forced to follow matching condition based on energy and mass conservation. Energy conservation requires,

$$[\mathbf{n} \cdot k \nabla T]_\Gamma = \dot{m} h_v \quad (13)$$

where h_v is the enthalpy of vaporization. For a multicomponent fuel, h_v is mass averaged based on the composition at the interface, that is

$$h_v = \sum_{x \text{ is Fuel}} h_{v,x} Y_x \quad (14)$$

Further, it is required that

$$[\mathbf{n} \cdot \rho D_x \nabla Y_x]_\Gamma = \dot{m} [Y_x]_\Gamma \quad (15)$$

is satisfied for each species. The combination of the temperature matching condition, fuel vapor matching condition, and the equilibrium relations (Raoult's and Clausius-Clapeyron) yields an eigenvalue problem that can be solved for the vaporization rate, $\dot{m}$.

C. Thermodynamic Equilibrium and Interface Conditions

In [2] three strategies were introduced to close the interface thermodynamic equilibrium problem in the context of a single component fuel. The MB strategy (based on [16]), was based on directly implementing and solving the eigenvalue problem. This strategy is the most intuitive, and it may be the most sound modeling approach. However, the strategy suffers from both low numerical accuracy and a computationally expensive implementation. The REA strategy (based on [17]) forgoes solving the eigenvalue problem. Instead a low order estimate of the solution is made, and then a correction is added for any error in conservation. The REA2 strategy is similar but uses a second order estimate rather than a first order estimate. The REA2 method was found to be the most accurate of the three strategies, however, did not produce great computational expense.

The strategy used in the current work is an extension of the REA2 strategy. The original strategy worked by extrapolating the mass fractions from the gas phase to the liquid-gas interface, and then inverting the Clausius-Clapeyron relation to find the interface temperature. This strategy extends naturally to multicomponent fuels with one important modification. For a multicomponent fuel, the problem of finding the temperature by inverting Eqs. (11) and (12) is overdetermined and must be solved using a least squares strategy. The equation solved is,

$$T_{\Gamma} = \operatorname{argmin} \sum_{x \text{ is Fuel}} \left(\chi_{G,x} - \chi_{L,x} \exp \left[-\frac{h_{v,x} W_x}{R^o} \left(\frac{1}{T} - \frac{1}{T_{b,x}} \right) \right] \right)^2 \quad (16)$$

which can be solved using any algorithm for finding minima. Golden section search [18] was used here.

This strategy for interface thermodynamic equilibrium is *ad hoc*, and its thermodynamic implications will be explored further in future work. For this work, a few trends were noted which gave confidence in the strategy for initial investigations. When used with a single component fuel, the strategy (Eq. (16)) yielded the same value as using a standard root finder. However one important note is that solving for a root using Eq. (16) was significantly slower than using a root finder. Even considering a root finder that has the same theoretical convergence rate as golden section search. Another note was that for multicomponent mixtures, Eq. (16) seems to always yield an interface temperature that is lower than the max $T_{b,x}$ and at least as high as min $T_{b,x}$ which agrees with intuition.

IV. Vaporizing & Atomizing Jet

This work involved some exploratory simulations of a vaporizing spray jet. To minimize the cost of these initial simulations, the study was performed in two dimensions. The liquid properties of the jet correspond to those given in Table 2 for the tri-component surrogate. The gas properties are also the same, except the gas density which has been increased to 72.8 kg m^{-3} to emulate the high pressure environment inside the gas turbine. A jet of diameter 1.3 mm is injected in a domain much larger than itself, $31.2 \text{ mm} \times 10.4 \text{ mm}$. The domain has an ambient gas at temperature 1500 K and velocity of 15.8 m/s in the positive x direction (*i. e.* towards the right). The jet is injected with interface conditions (see Section V), and it has velocity 12.8 m/s in the positive y direction (*i.e.* vertically). This results in a momentum flux ratio, $q = 6.6$, which is chosen to be similar to non-vaporizing simulation of [19]. Despite the similarity in q , the simulations are not directly comparable. In particular, the pattern of droplet breakage and the droplet size distribution look different. This is not entirely surprising. First, the current simulation is performed in two dimensions whereas Herrmann's work is three dimensional. The processes of wake vortex formation and dissipation are quite different between these types of flows. Second, and perhaps more importantly, this exploratory study was done with a fairly low mesh resolution.

A snapshot of the jet was shown in Fig. 1. The liquid-gas interface can be visualized as gray contour in the flow. Ideally a visual interpretation of the composition that is simple to interpret like the temperature plot could be used. It is challenging in general to visualize high-dimensional data such as the composition of the vapor in a multicomponent fuel blend. However, for the specific case where three (or fewer) species exist, the vapor fields can be simultaneously visualized using the following method. The key to this visualization is noting that there exist three primary colors, hence each field can be associated to an intensity of one of the three colors. Through some experimentation, it was found that the additive primary colors (Red, Green, and Blue) tend to render poorly. Since most of the vapor lies near the jet, the majority of the computational domain is pure air. Using the RGB scheme for such a situation yields an image that is nearly all black, except near the jet. Interestingly, this color scheme also has the property that regions of the flow with high concentrations of fuel vapor become white. Accordingly, the subtractive primary color scheme (Cyan, Magenta, Yellow) was used instead. This results in images that are white in regions where no vapor lies, and become darker in

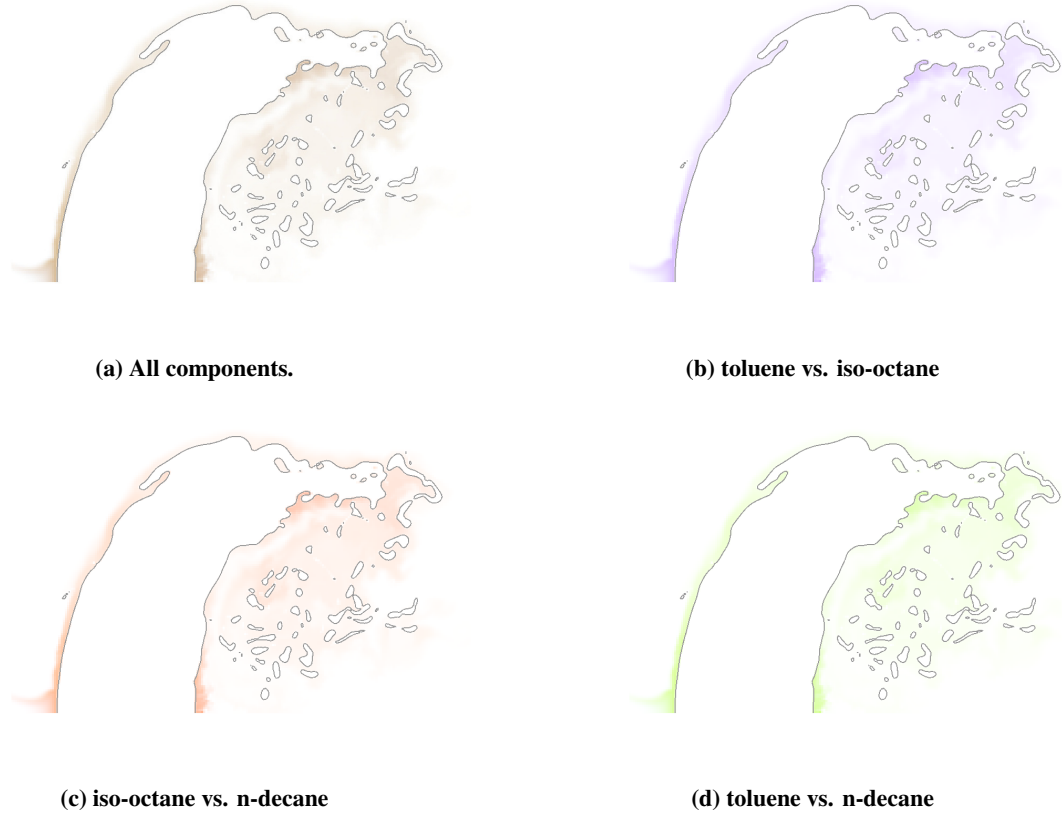


Fig. 2 Composition of vaporizing and atomizing jet. The gray contour is the liquid-gas interface.

color as the concentration of vapor increases. They are demonstrated below in Fig. 2 where color scheme refers to toluene (C), iso-octane (M), n-decane (Y). A CMY colormap is included as visual aid Fig. 3.

Unfortunately, when all three colors are plotted together Fig. 2a, the mixture of the three colors leads to images that are all brown/black in color. This unsurprising given the color map (Fig. 3), however, the similar hues and darkness demonstrated by these mixtures makes interpretation of results more challenging. Results are much easier to interpret using the binary plots of species against species. Using Fig. 3 as an aid, Fig. 2b demonstrates a color that is closer to Magenta than Cyan. Accordingly, there is more iso-octane in the vapor than toluene. Similar analysis of the Fig. 2d demonstrates that there is also considerably more n-decane in the vapor than toluene. Figure 2c suggests more n-decane than iso-octane in the vapor, however, the distribution is more even than the toluene/iso-octane and toluene/n-decane plots. This conclusion is very interesting, because iso-octane is actually the most volatile species and n-decane is the least volatile species. A commonly held belief is that the most volatile species will vaporize the most, and other species will follow in order of the volatility. Here, a different trend is seen. However, this trend can be justified in light of Raoult's law Eq. (11). The law predicts that the amount of vapor depends on both the natural volatility of the species (via $\chi_{G,x}^*$) and the concentration of the species in the liquid phase. Even though n-decane is the least volatile species, it has the highest concentration in the liquid phase. Hence, it appears at the highest concentration in the overall vapor.

Despite this it can be seen that diameter of the smallest droplets is quite small compared to that of the spray jet. The smallest structure noted in the mesh has a diameter slightly smaller than that of the mesh size. Such a structure cannot be well-captured on the mesh, and accordingly, the predictions of vaporization and mixing that are occurring around this structure cannot be accurately captured. Since the structure is too small to be captured, introduction of appropriate submodels would be appropriate. For this reason strategies that combine elements of interface-capturing study and Lagrangian particle modeling such as [19] may be important tools for research in the near future. The rest of the paper is dedicated towards study of droplets, with the aim of improving the state of the art in Lagrangian modeling.

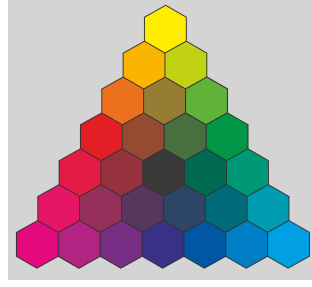


Fig. 3 CMY Color Table via *Wikimedia Commons*

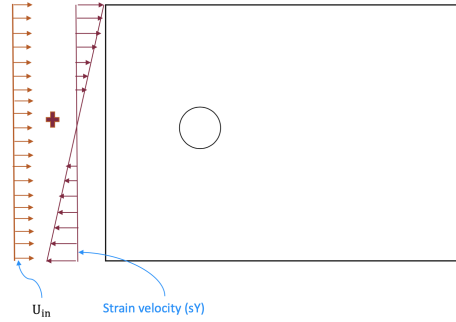


Fig. 4 Cartoon of simulation domain approach. A zero pressure gradient inlet with mean velocity U_{in} and strain velocity S_y depicted. The inlet is paired with a convective outflow (on the right). The other boundaries are free-slip (zero normal gradient).

V. Droplet Test Configuration

Tests will study the process of preferential vaporization of the multicomponent fuel droplet and compare to a reference single component fuel. The reference single component fuel is n-dodecane which is a jet fuel surrogate. The test configuration used for this study has been used previously by the PI's group [20, 21], and it is depicted in Fig. 4. We study the vaporization of a single droplet in a gaseous flow. The configuration also allows for the study of non-uniform flows such as those in turbulent flow by introducing a linear shear to the velocity. This approach is based on the assumption that the typical droplet is as small as (or smaller than) the Kolmogorov turbulent length scale. Under that assumption, the effect of turbulence is well-approximated by a droplet in a simple shear flow. A critical part of this set up is the fact that the droplet is not suspended using wires or fibers, and accordingly, an accurate understanding of droplet internal circulation can be reached. To ensure that the droplet remains centered in the computational domain, the configuration mimics a droplet falling at terminal velocity by imposing an artificial gravitational acceleration. By altering this acceleration, studies can be run of droplet vaporization at arbitrary inflow velocity.

The study will compare the influence of various non-dimensional groups on the vaporization of the fuel species. The relevant quantities are

- 1) The Reynolds number, which demonstrates the boundary layer evolution, $Re = \rho_G U_\infty d \mu_G$
- 2) The Weber number, which demonstrates the relative influence of aerodynamic-to-surface tension forces, $We = \rho_G U^2 d / \sigma$. It indirectly quantifies the shape of the droplet. As Weber approaches zero, the interface shape approaches a sphere. In the opposite limit, the droplet deforms to more complex shapes.
- 3) The gas density itself, which changes considerably between the atmospheric conditions experienced in laboratory and the in-flight conditions. The ratio $\Lambda = \frac{\rho_L \mu_L}{\rho_G \mu_G}$ is more useful to know theoretically because it can be shown that this quantity relates to the droplet's internal circulation [22]. For this study we define, $\hat{\Lambda} = \Lambda_{ATM} / \Lambda$, the ratio of the current Λ its value at atmospheric conditions.
- 4) The strain rate, S . The strain rate allows a representation of flow non-uniformity. For a turbulent flow with kinematic viscosity, ν and Kolmogorov length scale, η , the mean strain rate can be shown to be $S = \nu / \eta^2$. Assuming the droplet satisfies, $d \sim \eta$, a relationship for the strain rate can be formed. The strain rate can be non-dimensionalized

Case	Re	We	$\hat{\Lambda}$	$\hat{S}$
01	12	1	1	0
02	60	1	1	0
03	60	1	40	0
04	60	8	40	0
05	60	1	1	0.1
06	60	1	40	0.1

Table 1 Test Matrix

as $\hat{S} = Sd/U_\infty$.

The test matrix is demonstrated in Table 1. The initial droplet size is $100\mu m$. The domain is of size $2.4d$ in all three spatial dimensions, with a mesh resolution of $N = 40$ grids in each direction. From experience, this domain size and resolution are known to be sufficient to analyze trends about the droplet behavior.

Using the physical properties of air (Table 2), the velocity of air is determined to achieve the target Reynolds number. The Weber number is manipulated by altering the liquid surface tension. Since it is expected that the surface tension is only important insofar that it affects Weber number, this is assumed to be a reasonable manner to study this phenomenon. To study the internal circulation, the gas density was modified to achieve the given value of $\hat{\Lambda}$. The value of $\hat{\Lambda}$ used here was chosen to replicate the physical process of operation in a gas turbine engine. In that context, the engine pressure may be as high as 50 times that of atmospheric pressure. However, to ensure that this does not alter the Reynolds and Weber numbers, the droplet diameters were decreased such that $\rho_G d$ remained constant in all cases.

A. Boundary Conditions, Initialization, and Fluid Properties

The domain is set up with an inlet boundary condition on the left (negative x direction), and an outlet on the right (positive x direction). The top and bottom (positive and negative y directions) use a free-slip boundary condition. The simulation is periodic in the z direction. The inlet boundary value of temperature is $1500K$ and the gas is assumed to be pure air at the inlet. The gas in the computational domain is initialized with the temperature and species fractions profile from the d^2 law analytical solution to droplet vaporization [4]. The liquid is assumed to be preheated to the interface temperature, and the tricomponent mixture is assumed to be perfectly mixed. From the assumption of a freestream temperature of $1500K$ and a pure air freestream, the necessary values of species mass fraction and temperature at the liquid-gas interface can be computed. In this case, two sets of simulations were performed, one for the tricomponent fuel surrogate [10] and the other for n-dodecane. Since the thermochemical properties of these two jet fuel surrogates are different, we recover different properties for the interface. Noting this fact is important for the interpretation of the results in this work.

The fluid properties are listed in Table 2. The bulk of each phase is treated as a fluid with constant properties. However, to more accurately simulate species diffusion, mixing, and multicomponent vaporization this assumption was not used for all aspects of the problem. Computations involving diffusion rates, molar masses, boiling temperature, and vaporization enthalpies use the values of the constituent species as appropriate. Since the mass diffusion rates in the liquid are very small, $\sim 10^{-10}$, they are set to zero for these simulations. Accordingly, only the effects of advection are seen in the liquid phase transport. It will be shown as part of the work, that this transport is significant. Fluid properties are taken from two sources. Fuel properties are taken from Yaws' handbook [23] and air properties are taken from the Engineering ToolBox [24].

VI. Droplet Results

A. Vaporization Rate

The primary target of this work was to understand how the conditions affected the vaporization rate of the droplet. This is demonstrated in Fig. 5. Historical knowledge and analytical theory, i.e. the d^2 law, suggest best practices for displaying this information [4]. In this case, the instantaneous droplet diameter is taken to be the diameter of a spherical

Property	Gas	Liquid (tricomponent)	Liquid (n-dodecane)
ρ	1.77	728	745
μ	1.846e-5	8.632e-4	0.001390
c_p	1004.9	2204.8	2210.78
λ	2.218e-5	8.2923e-8	8.3e-8
σ	—	0.02341	0.02494

(a) Bulk fluid properties

Property	toluene	iso-octane	n-decane	n-dodecane
h_v	364550	271560	281260	260306
M	0.092141	0.11423	0.14229	0.170338
T_b	383.78	372.39	447.3	489.47
D	8.49e-6	6.32e-6	5.35e-6	4.73e-6

(b) Vaporization properties

Table 2 Fluid properties

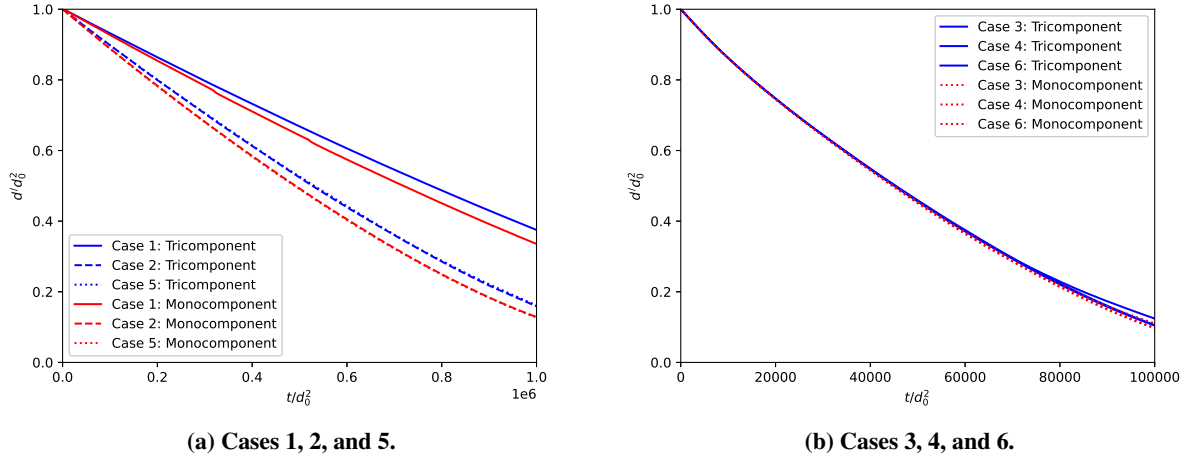


Fig. 5 d^2/d_0^2 against t/d_0^2 .

droplet with the same volume. A general trend is seen that the monocomponent surrogate (n-dodecane) vaporizes faster than the tricomponent surrogate. This is largely due to the higher equilibrium temperature of the monocomponent surrogate. In practice, the interface temperature of the monocomponent droplet equilibrates to a temperature slightly below the boiling temperature of the liquid phase. For the monocomponent droplet, this value is given by n-dodecane (489.47 K). However, for the tricomponent mixture, the equilibrium temperature is brought down by the lower boiling points of the constituent chemical species. In particular, the droplet equilibrates to a temperature that is between the boiling temperatures of iso-octane and n-decane, both of which boil at temperatures considerably lower than n-dodecane.

Other than this fact, the data for the monocomponent surrogate and the tricomponent surrogate appear to yield similar trends. Comparing Cases 1 and 2 yields the expected result that as Reynolds number is increased, the vaporization rate increases. This effect is established in the literature [25].

Comparing Cases 2 and 5 suggest the vaporization rate may be largely independent of strain rate. The lack of dependence of the vaporization on strain rate can be explained by defining a strain velocity, Sd . This quantify measures the effect of strain as it shows the velocity difference between the bottom and top of the droplet caused by flow non-uniformity. When $Sd \ll U_\infty$ the strain does not significantly alter the velocity over the surface of the droplet, and accordingly it does

not have a significant effect on the vaporization. In [20], it was discovered that large values of this quantity do indeed lead to significant enhancement of vaporization rate, at least for droplets in two dimensions. However, sustained strain at such rates are unreasonable in practice. This is because droplets tend to respond to high strains by breaking into smaller droplets. When the droplets are small enough so that break-up no longer occurs, the quantity, $\hat{S}$, becomes quite small.

Comparing Cases 2 and 3 suggest a strong dependence of results on internal circulation as the droplet in Case 3 vaporizes much quicker in scaled time, t/d_0^2 . Strictly, speaking it needs to be established that $\hat{\Lambda}$ relates to the internal circulation. Several methodologies for quantifying internal circulation are discussed and evaluated in [21]. And that paper demonstrates that the gas density does indeed control internal circulation. For ease of explanation, the quantity chosen in this work is the enstrophy, defined,

$$\mathcal{E} = \frac{1}{V_L} \int_L \frac{1}{2} \omega^2 dV \quad (17)$$

where ω is the vorticity and the integral is taken over the liquid. That is, the enstrophy is half of the mean square vorticity. From dimensional analysis, the enstrophy should scale as

$$\mathcal{E} \sim \frac{U^2}{d^2} \quad (18)$$

Given that the velocity is the same in both cases, naïve scaling suggests,

$$\mathcal{E}_3 \sim \left(\frac{d_2}{d_3}\right)^2 \mathcal{E}_2 = 1600\mathcal{E}_2 \quad (19)$$

However, this property was not recovered. Case 2 reached peak values on the order of $2 \times 10^7 s^{-2}$ whereas Case 3 reached values of $3 \times 10^{11} s^{-2}$, which greatly exceeds the value from the naïve scaling. This is not surprising, as the internal circulation parameter $\hat{\Lambda}$ has changed between the two simulations, or equivalently that $\Lambda_3 < \Lambda_2$. This suggests that changing Λ is in fact a good predictor for changing internal circulation, and agrees with [21]. With this information, it appears that the difference in vaporization rate between Cases 2 and 3 is explained by internal circulation. This is an interesting discovery since the droplets were preheated in these simulations. Therefore the internal circulation must be affecting the vaporization through a mechanism that is more complex than simply affecting the liquid heating rate. It is postulated that the internal circulation affects the thickness of boundary layers near the interface. This in turn affects the mass transfer between phases and ultimately the vaporization. However, this phenomenon should be studied in further detail.

Comparing Case 3 and 4 suggest a lack of dependence of vaporization rate on Weber number. The lack of Weber number dependence seems to contradict previous research which has demonstrated that increasing the Weber number of droplets leads to increasing the vaporization rate of droplets [6, 26]. However, this previous research was performed for droplets in the limits of $We \rightarrow 0$, $Re \rightarrow 0$, and no internal circulation. The physics of that type of flow is considerably different than that of the current problem. In particular, significant boundary layer separation and wake vortex generation occurs in the current flow. The internal circulation inside of the droplet is also significant. These flow phenomena generate a more complex nonlinear response of vaporization behavior with Weber number. Accordingly, the more simple flow theory may not apply in all circumstances, for the more complex flows seen here.

B. Refined Simulations

A second set of simulations was performed with slightly larger domain and finer mesh resolution. The goal of this second set of simulations was to better understand the effect of the droplet internal motion on the flow, and to better capture what happens in the wake region behind the droplet. The domain was sized $4.8d \times 2.4d \times 2.4d$ and a $128 \times 64 \times 64$ grid was used. To understand the importance of internal circulation, two initial conditions were compared for the tricomponent surrogate. The uniform initialization, which was used for the previous studies, was used. In addition to this condition, a “shell” initialization was used. A commonly used model of droplet vaporization holds that the fuel components vaporize in order from most to least volatile as if they were organized as concentric shells of fuel. This initialization considered the case were the droplet truly had such a shell structure, Fig. 6. The remaining parameters are the same as Case 2.

Relevant information is demonstrated in Fig. 7. For the course of the simulation, the rate of vaporization is fairly similar (Fig. 7a). One interesting trend is the interface temperature for the shell case. For the shell case, the interface

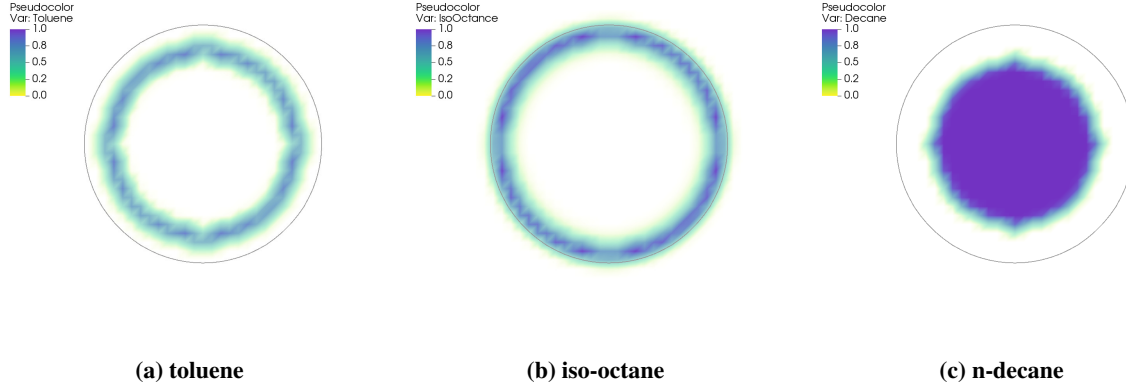


Fig. 6 Shell initialization.

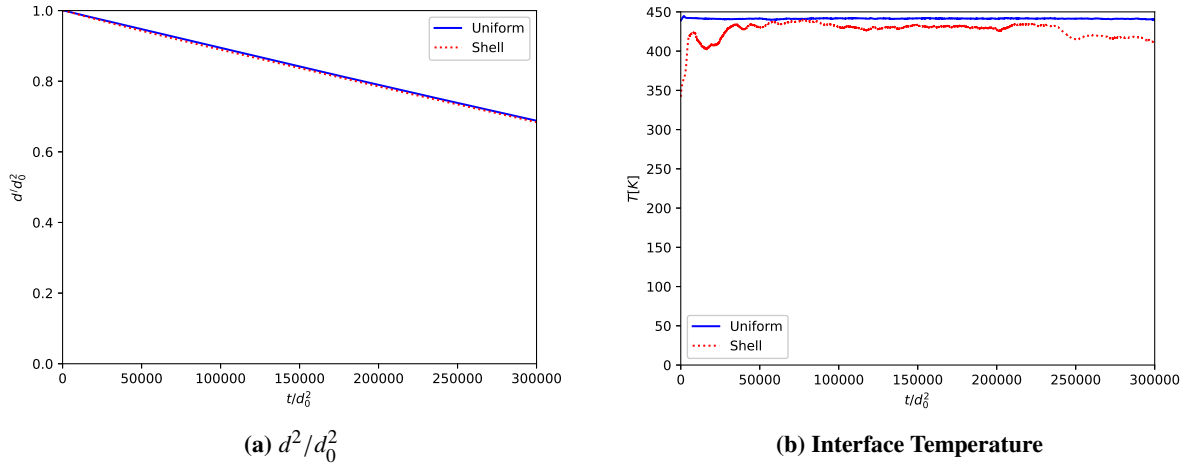


Fig. 7 Liquid initialization effects on vaporization.

temperature begins at the boiling point of the most volatile component, iso-octane. Over the course of the simulation, it rapidly increases towards that of n-decane (the least volatile component). Accordingly, it approaches the same value as that seen in the uniform case. Although, it is important to point out that in the current case, the composition of the liquid is not uniform. Accordingly, it is unclear what is the appropriate interpretation of the interface average values demonstrated in Fig. 7b.

The internal circulation inside the droplet is significant in this problem, and causes significant transport of the liquid species (Fig. 8). It is important to recall, that the mass diffusivities in the liquid phase are set to zero, so this transport is entirely due to internal circulation. The vortex motion causes the formation of complex patterns in the species. It is immediately clear that the common assumption of spherically symmetric profiles inside the droplet is false. At this snapshot in time, n-decane seems to concentrate primarily in the front of the droplet, whereas iso-octane concentrates toward the rear. Toluene appears to lie in the region between the other two species. One interesting note is that despite the drastic changes in composition, the vaporization rates for the shell case and the uniform initialization are quite similar. This can be made even more precise by extracting the local vaporization rate $\dot{m}$ as in Fig. 9. The pseudocolor of $\dot{m}$ looks almost the same in both cases, implying that this quantity is not strongly related to the composition, at least for this case. From this, it may be concluded that the vaporization is strongly driven by the temperature, and is largely independent of the local species composition. However, it is interesting to note differences in the composition of the vapor between the two cases (Fig. 10). For the uniform initialization case, the vapor is fully mixed at the interface and also downstream. This is represented by the nearly constant brown color. For the shell initialization case, it is clear that the composition of the vapor changes around the droplet. Near the front of the droplet, the vapor is largely n-decane, which

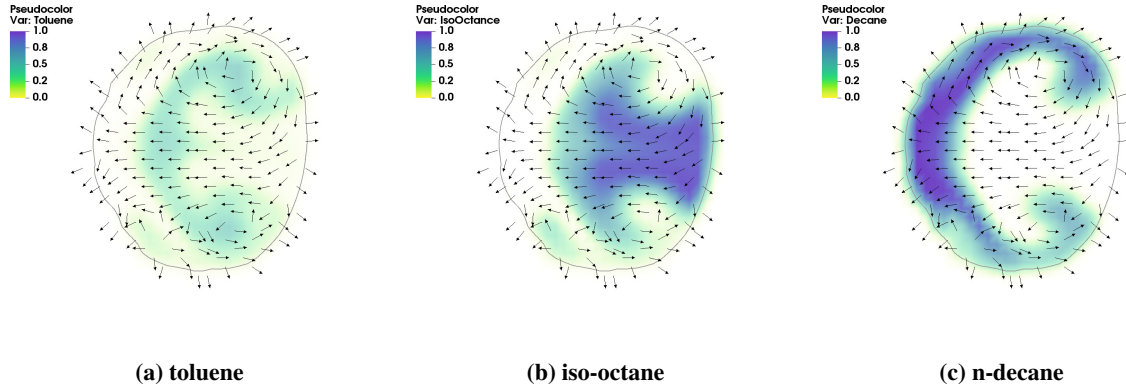


Fig. 8 Snapshot of liquid composition. The interface is demonstrated by a gray contour. The vectors are the velocity of the liquid.

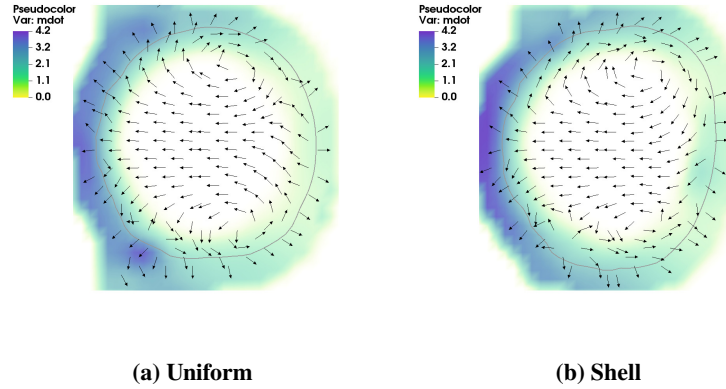


Fig. 9 Vaporization rate, $\dot{m}$. Smoothed. The interface is demonstrated by a gray contour.

is consistent with that region being where most of the n-decane liquid lies. Similarly, the region at the rear of the droplet is largely iso-octane. The figure also suggests that downstream of the droplet, mixing occurs. The implications for this type of segregation of vapor could be an interesting topic of exploration. OB

Over larger periods of time, the composition becomes largely uniform within the liquid droplet. As that occurs, the vapor field also becomes uniform. This was inspected by eye using images such as Figs. 7 and 10 taken as time series. For the given case, flow uniformity does not occur until a significant portion of the droplet has already vaporized, approximately 30% per volume.

VII. Conclusions

This work developed a strategy for interface-capturing direct numerical simulations of multicomponent fuel spray vaporization. The strategy was applied to look at an atomizing and vaporizing jet of multicomponent liquid in two dimensions. Some discussion about the vaporization rate behind the jet is given. One interesting fact was that for this simulation, the least volatile species was actually the most abundant in the vapor phase. This counterintuitive fact was linked to Raoult's law.

Although demonstrating that true direct numerical simulations of spray are possible, the work also laments the high computational cost of such simulations. For the near future, strategies such as [19] that combine direct numerical simulation with Lagrangian modeling will likely be the standard. The work then explores droplet vaporization to highlight phenomena that should be included as part of next generation Lagrangian models.

As is traditionally known, the Reynolds number is an important factor in predicting droplet vaporization. This work



Fig. 10 Vapor visualized using CMY scheme. The interface is demonstrated by a gray contour. (See Section IV for interpretation).

also demonstrated that the droplet’s internal circulation, reflected by the ratio Λ , is important towards predicting the vaporization rate of droplets. This is interesting since the droplets were preheated in this case, and therefore suggests that internal circulation must affect vaporization through a mechanism that is not directly related to droplet heating. Interestingly, no effects were found for the droplet shape as characterized by the Weber number. This seems to contradict previous work in the arena. However, since that previous work was performed for $Re \rightarrow 0, We \rightarrow 0$ limit, it could simply suggest that more complex interactions are relevant for the higher Reynolds numbers demonstrated in this work. The strain rate appeared to have no effect on vaporization rate, and hence the commonly used Lagrangian strategy of assuming the droplet experiences uniform flow seems justified. The single component fuel surrogate vaporized faster than the multicomponent fuel surrogate. Otherwise, there does not seem to be any significant difference in trend between the two surrogates.

Comparing a droplet initialized with a uniform species fields and “shell” fields demonstrated that vaporization seems to be almost independent of the composition. The results for the uniform case and the shell case were almost identical, even though the distribution of species in the liquid phase is quite different for the two cases. This is true, even though noticeable differences are seen in the vapor field, and suggests that the vaporization rate is largely driven due to temperature gradients. Over long periods of time, the internal circulation in the droplet causes the composition within the droplet to be uniform, which in turn, leads to a uniform composition of the vapor.

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