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REVIEW ARTICLE

Numerical Modeling of Evaporation and Combustion of Isolated Liquid Fuel Droplets: a Review

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Abstract | Understanding the transport processes during evaporation and combustion of isolated liquid fuel droplet is highly important in several applications involving sprays. Comprehensive numerical models assist in carrying out simulations involving interlinked transport processes in liquid and gas phases using proper interface coupling conditions. The predictions from such numerical models reveal flow, temperature and species fields, with which the evaporation, as well as combustion characteristics, can be thoroughly analyzed. In this article, a detailed review of numerical models used to simulate evaporation of isolated droplets under several operating conditions is presented. This includes evaporation in high-pressure conditions, where real gas effects and solubility of ambient gas into the liquid droplet, come into play. Subsequently, a review of droplet combustion models, which are comprehensive enough to reveal the burning characteristics of an isolated droplet, is presented. Importance of liquid phase motion on evaporation and combustion behavior and water absorption in the case of alcohol droplets are reported. This review also includes modeling concepts applied to multi-component droplets.

Keywords: *Isolated droplet, Evaporation and combustion, Liquid-phase motion, Marangoni convection, Interface coupling, High-pressure evaporation model, Ambient gas solubility*

1 Background

In the sparse region of a liquid fuel spray, individual droplets move towards the combustion zone at different velocities and undergo evaporation and/or combustion under different ambient conditions. Interaction between the droplets in the sparse region is expected to be minimum. Further, studies on liquid fuel characterization are conducted on individual droplet using different techniques such as suspended droplet, freely falling droplet and porous sphere method. Therefore, the study of evaporation and combustion of isolated liquid fuel droplets under several operating conditions is of critical importance and forms the first step towards considering a spray model.

Periodically, extensive reviews on evaporation and combustion of droplets have been reported in the literature. These include the reviews by Williams[1], Faeth[2], Law[3], Faeth[4], Sirignano[5], Dwyer[6], Law and Faeth[7], Givler and Abraham[8], and Birouk and Gökalp[9]. Different aspects of droplet evaporation and combustion, analyzed using different methodologies, experimental, theoretical and numerical, have been reported in these reviews.

Droplet evaporation: phase change occurring at the surface of a liquid fuel droplet.

Most of the numerical studies on droplet evaporation and combustion invoke an assumption of droplet remaining spherical throughout its lifetime, considering low values of Weber number. Comparison of predictions from these models with experimental results has shown promising trends. In general, a numerical simulation should be capable of reporting detailed flow filed, species and temperature distribution, which are difficult to measure even using complex experimental techniques. Such a comprehensive numerical

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model includes governing equations for flow, species and energy in liquid phase and gas phase, solved in a decoupled manner, and uses interface coupling conditions to couple these solutions. Numerical models, which use two-phase models such as volume of fluids (VOF) and level set methods, and solve the transport equations inherently considering the exchanges of mass, momentum, species and energy between the phases, are also available in the literature. An exclusive review of numerical modeling of evaporation and combustion behavior of isolated fuel droplets will be useful in understanding the assumptions, simplifications and model parameters required for comprehensive modeling of the transport processes involved during evaporation or combustion of droplets. In this review, details of numerical works reported on evaporation and combustion of liquid fuel droplets are presented systematically.

Interface coupling: conditions prescribed for exchange of mass, momentum and energy between liquid and gas phases.

2 Numerical Formulation for Evaporation and Combustion of Spherical Droplets

In this section, a general numerical formulation for simulating the evaporation and combustion characteristics of spherical liquid fuel droplets is presented. Incompressible and laminar flow are assumed. Several one-dimensional (radial flow) models are reported to simulate the spherically symmetric process. Several axisymmetric models have been considered to account for non-spherical gas phase over a spherical droplet. The thermophysical properties are evaluated as a function of pressure, temperature and composition of the mixture. The governing equations are listed below.

Using the density of the mixture, ρ, and mixture velocity vector ($\boldsymbol{V}$), the continuity equation in the liquid and gas phases is written in the following equation:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{V}) = 0. \tag{1}$$

For ith species in the mixture, the conservation equation in terms of its mass fraction, Y_i, its (species) velocity ($\boldsymbol{V_i}$) and its net rate of production, ω_i, is written in the following equation:

$$\rho \frac{\partial Y_i}{\partial t} + \rho \boldsymbol{V} \cdot \nabla Y_i = \omega_i - \nabla \cdot (\rho Y_i \boldsymbol{V_i}). \tag{2}$$

The species velocity ($\boldsymbol{V_i}$) is determined using Stefan–Maxwell equation, including the Soret effect, or using any simplified approach. For evaluating the net rate of production of the ith species, ω_i, a reaction scheme is selected. This may be as simplified as a global single step reaction or even a detailed kinetics mechanism. If there are multiple components (N), then ($N-1$) species conservation equations are solved. In the liquid phase, if more than one component is present, then species conservation equation is solved for all components, leaving one of the component. In liquid phase, the net rate of production of species is not included in the governing equation.

Detailed kinetics: a reaction mechanism that incorporates several elementary reactions and minor and major reacting species to predict the reaction rates.

Momentum conservation equation for both phases is written in the following equation, using pressure (p) and velocity gradients:

$$\frac{\partial}{\partial t}(\rho \boldsymbol{V}) + \nabla \cdot (\rho \boldsymbol{V}\boldsymbol{V}) = -\nabla p - \nabla\left[\frac{2}{3}\mu(\nabla \cdot \boldsymbol{V})\right] + \nabla \cdot \left(\mu\left[(\nabla \boldsymbol{V}) + (\nabla \boldsymbol{V})^T\right]\right) + \rho \boldsymbol{g} - \rho\frac{\mathrm{d}U_\infty}{\mathrm{d}t}. \tag{3}$$

Here, the last term in the right-hand side includes the deceleration of a moving droplet due to the drag in the gas phase. While simulating suspended or stationary droplet, this term is not considered. Similarly, the buoyancy term (fourth term in RHS) is not included for zero gravity conditions. In the liquid phase, this term is usually neglected.

The energy conservation equation for a reacting flow is written in the following equation in terms of temperature (T), using thermal properties such as thermal conductivity (k) and specific heat (c_p):

$$\frac{\partial}{\partial t}(\rho T) + \nabla.(\rho \boldsymbol{V} T) = \nabla.\left(\frac{k}{c_p}\nabla T\right) + \frac{k}{c_p^2}\nabla T.\nabla c_p - \frac{1}{c_p}\sum_{i=1}^{N}\omega_i h_i - \frac{\rho}{c_p}\sum_{i=1}^{N} Y_i \boldsymbol{V}_i.\nabla h_i + \frac{\dot{q}_R'''}{c_p}. \tag{4}$$

This includes enthalpy transport due to species diffusion (fourth term in RHS) and source term due to chemical reaction (third term in RHS) and a proper radiation model (last term in RHS). In the case of droplet evaporation, the chemical reaction term, ω_i, is set to zero. Similarly, for the liquid phase, chemical reaction and radiation terms are excluded.

These governing equations are coupled with a set of interface boundary conditions, which are given for (r, θ) coordinates, as follows:

At the interface, the gas and liquid phase temperatures are the same, as given in the following equation:

$$T_{\mathrm{g,s}} = T_{\mathrm{l,s}}, \tag{5}$$

where the subscripts, g and l, represent the gas and the liquid phases, respectively, and the subscript, s, denotes the droplet surface. The no-slip condition at the droplet surface requires the tangential component of velocity (v_θ) of gas and liquid phases to be same at the interface, as written in the following equation:

$$v_{\theta,\mathrm{g,s}} = v_{\theta,\mathrm{l,s}} \tag{6}$$

The mass flux ($\dot{m}''_\theta$) along the droplet surface is given in the following equation:

$$\dot{m}''_\theta = \rho_{\mathrm{g,s}}\left(v_{\mathrm{r,g,s}} - \frac{\mathrm{d}R}{\mathrm{d}t}\right) = \rho_{\mathrm{l,s}}\left(v_{\mathrm{r,l,s}} - \frac{\mathrm{d}R}{\mathrm{d}t}\right), \tag{7}$$

where $\mathrm{d}R/\mathrm{d}t$ is the droplet regression rate. Continuity of shear stress at the droplet surface includes the gradient of the surface tension (σ) and is given in the following equation:

$$\begin{aligned}&\mu_{\mathrm{g,s}}\left[\frac{\partial v_\theta}{\partial r} + \frac{1}{r}\frac{\partial v_\mathrm{r}}{\partial \theta} - \frac{v_\theta}{r}\right]_{\mathrm{g,s}} \\ &\quad = \mu_{\mathrm{l,s}}\left[\frac{\partial v_\theta}{\partial r} + \frac{1}{r}\frac{\partial v_\mathrm{r}}{\partial \theta} - \frac{v_\theta}{r}\right]_{\mathrm{l,s}} - \left.\frac{1}{r}\frac{\partial \sigma}{\partial \theta}\right|_{\mathrm{s}}.\end{aligned} \tag{8}$$

Species conservation at the interface is given in terms of convective and diffusive fluxes using radial diffusion velocity (V_r) in Eqs. (9) and (10).

For fuel components:

$$\begin{aligned}&\dot{m}''_\theta Y_{1,\mathrm{g,s}} + \rho_{\mathrm{g,s}} Y_{1,\mathrm{g,s}} \mathbf{V}_{\mathrm{r,1,g,s}} \\ &\quad = \dot{m}''_\theta Y_{1,\mathrm{l,s}} + \rho_{\mathrm{l,s}} Y_{1,\mathrm{l,s}} \mathbf{V}_{\mathrm{r,1,l,s}}\end{aligned} \tag{9}$$

For non-fuel components:

$$\dot{m}''_\theta Y_{\mathrm{i,g,s}} + \rho_{\mathrm{g,s}} Y_{\mathrm{i,g,s}} \mathbf{V}_{\mathrm{r,i,g,s}} = 0 \tag{10}$$

Here, subscript 1 represents the first fuel component and i represents the ith non-fuel component in the multi-component mixture. The conservation of energy at the interface requires balancing the heat conducted into the liquid phase, the heat conducted from the gas phase, the energy transported by the species and the energy required for phase change, given in terms of latent heat of vaporization (L). This is given, for a two-component fuel droplet, in the following equation:

$$\begin{aligned}&\dot{m}''_\theta\left(Y_{1,\mathrm{l,s}}L_1 + Y_{2,\mathrm{l,s}}L_2\right) \\ &\quad + \rho_{\mathrm{l,s}}\left(Y_1 \boldsymbol{V}_{\mathrm{r},1}L_1 + Y_2 \boldsymbol{V}_{\mathrm{r},2}L_2\right) \\ &\quad - k_{\mathrm{g,s}}\left.\frac{\mathrm{d}T}{\mathrm{d}r}\right|_{\mathrm{g,s}} = k_{\mathrm{l,s}}\left.\frac{\mathrm{d}T}{\mathrm{d}r}\right|_{\mathrm{l,s}}.\end{aligned} \tag{11}$$

For low–moderate pressure conditions, the equilibrium composition at the interface is calculated using Raoult's law expressed in terms of mole fraction, x, as in the following equation:

$$x_{i,g} = \gamma_i x_{i,l}\frac{p_i}{p}, \tag{12}$$

where p is the total pressure (atmosphere pressure), p_i is the vapor pressure of fuel species i evaluated using the equation such as Wagner equation, γ_i is the activity coefficient of fuel species i, which is evaluated using several methods, including the UNIFAC group contribution method.

For high-pressure conditions, fugacity values in liquid and gas/vapor phases for each species are equated as written in the following equation:

$$f_i^\mathrm{v} = f_i^\mathrm{l} \text{ or } y_i\phi^\mathrm{v} = x_i\phi^\mathrm{l}, \tag{13}$$

where f and ϕ are fugacity and fugacity coefficient, respectively, y and x are the mole fractions in gas and liquid phases, respectively, subscript, i represents ith species, and superscripts, v and l, represent vapor and liquid phases, respectively. A real gas equation of state, as presented in Eq. (14), is employed for fugacity coefficient calculation.

$$p = \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2} \tag{14}$$

The constants, a and b, take values depending upon the formulation and R is universal gas constant.

Based on the conditions, a numerical model can be used to solve for quasi-steady behavior during droplet evaporation or combustion. It is known that, for most of the fuel droplets excluding the multi-component droplets having components of widely differing volatilities, after a short initial transient period, the droplet surface regresses almost at a steady rate, as described by the d^2-law. During this quasi-steady evaporation or combustion, conservation equations for flow, energy and species are solved only in the gas phase along with appropriate coupling conditions for heat, mass and species balances at the liquid–gas interface. Here, liquid phase regression is not accounted for. This model applies to steady evaporation and burning, as in the case of porous spheres, where the liquid fuel is fed into the porous sphere at the rate equal to the rate of evaporation or burning.

Apart from the above approaches, a coupled two-phase approach that includes interface tracking using VOF or level set methods, has also been used for simulating droplet evaporation and combustion. This approach can handle droplet deformation. To model droplet deformation, generally a three-dimensional domain is involved, thus, it is highly computationally intensive.

3 Numerical Research on Droplet Evaporation

During the past decades, several numerical studies have been conducted on evaporation of liquid fuel droplet at atmospheric sub-critical, critical and super-critical ambient conditions, under micro and normal gravity, and at various convective fields. The major amount of work has been reported on the evaporation of low hydrocarbon liquid fuels (up to *n*-decane) and a few studies are also available on the evaporation of heavier liquid fuel droplets. There are several numerical studies on multi-component fuel droplet evaporation as well.

3.1 Numerical Models for Evaporation Under Low–Moderate Ambient Pressures

Several studies investigated the evaporation of liquid droplets within low-pressure environments; most of the studies assumed that the droplets maintain a spherical shape. Tong and Sirignano[10] developed a simplified model for multi-component transient fuel droplet vaporization in a hot convective environment. A steady convective gas phase analysis was carried out using a similarity transformation together with a stream function like simplification. The model included features such as liquid phase internal circulation, transient droplet diffusion and axisymmetric gas phase convection. Gogos and Ayyaswamy[11] developed a model to study the evaporation of slow-moving droplets. The flow in the gas phase and the droplet internal circulation were treated as steady. The droplet heating was time dependent. Aharon and Shaw[12] investigated the influences of thermal and solutal Marangoni effects on the hydrodynamic stability of binary droplets, evaporating in a hot environment. They used a linear stability approach for this analysis. They analyzed the stability of alkane–alkane and alcohol–water mixtures. They concluded that the thermal Marangoni effect (surface tension gradient due to temperature gradient) had a stabilizing effect and the solutal Marangoni effect (surface tension gradient due to composition gradient) had a destabilizing effect. However, they have not considered the effect of forced convection on the Marangoni instability of the droplet. In addition, their analysis did not take into account the deviation from ideality of the bi-component mixture.

Ha and Lai[13, 14] used linear stability analysis and energy method to study the Marangoni instability of a vaporizing droplet. They developed a simplified model to predict the critical thermal and solute Marangoni numbers. A model for unsteady droplet vaporization for a wide range of temperatures was developed by Ra and Reitz[15]. An unsteady internal heat flux model and a method to determine droplet surface temperature were proposed in their work. Tonini and Cossali[16] developed a new analytical model to study liquid droplet evaporation in gaseous environment, which was valid for a wide range of conditions, based on the solution of species, momentum and energy conservation equations in radial coordinates. Fairly good predictions were achieved by this model when compared to other models. Most of these analytical models, however, were not capable of predicting the transient nature of flow taking place within the droplet.

Law[17] developed a model for the vaporization of a miscible multi-component droplet with the following assumptions: transient diffusion within the droplet, quasi-steady diffusive-convection in the gas phase and ideal behavior of the mixture. Abramzon and Sirignano[18] developed a simple, but sufficiently accurate procedure for spray combustion calculations. Their model considered variable thermophysical properties, non-unit Lewis number in the gas film, Stefan flow, internal circulation and transient heating in the liquid phase. They formulated a simplified, one-dimensional, effective conductivity model for transient liquid heating with internal circulation. They used one-dimensional 'stagnant film theory' for the gas phase, which included the Stefan flow effect. Using their model, they studied vaporization characteristics of droplets injected into steady/fluctuating hot air streams.

Haywood et al.[19] investigated isolated droplet vaporization using transient two-phase model and predicted the internal temperature distribution within the droplet. They included the effects of variable thermophysical properties, heating and flow in the liquid phase and transient variations of droplet size and velocity in their model. However, they have not studied the effect of surface tension variation along the droplet surface on the droplet internal flow field. Megaridis and Sirignano[20, 21] simulated bi-component droplet vaporization by numerically solving the Navier–Stokes equations in an axisymmetric geometry. Their study showed preferential vaporization of the more volatile species and that when a part of the most volatile species was trapped inside the recirculation zone, the lesser volatile species evaporated faster.

Chiang et al.[22] analyzed the evaporation characteristics of a cold fuel drop injected suddenly into a hot ambient. The features of their model included variable thermophysical properties, transient heating, internal circulation, drag experienced by droplet, boundary-layer blowing and moving interface. They studied the effects of varying the transfer number on the vaporization rate and the drag coefficient. They found that for higher transfer numbers, the evaporation rate was higher and for lower transfer numbers, the boundary-layer blowing effect was weak. They obtained correlations for drag coefficient, Nusselt and Sherwood numbers from a large amount of numerical data. Their work concentrated more on the dynamics of the droplet, however, without considering surface tension induced flow within the droplet. Megaridis[23] studied the vaporization of a multi-component droplet under laminar convective environment. Effect of convection on droplet internal flow, however, was not studied. Megaridis[24] used variable properties in the liquid phase to simulate droplet vaporization and found that the mixture density variation was more critical than the heat capacity variation.

Renksizbulut and Bussmann[25] developed a numerical model considering transient effects for droplet size and velocity variations, heat and mass transfer within the liquid phase and thermophysical properties varying as a function of temperature and concentration in both phases. Using their model, they studied the convective evaporation of *n*-decane + *n*-hexadecane droplet in air at 1000 K and 10 atm with Reynolds number of the order of 100. Their model considered vapor–liquid equilibrium at the interface using Raoult's law. Haywood et al.[26] developed a numerical model to predict the transient droplet size, velocity, pressure, temperature and concentration fields in both liquid and gas phases. They used this model to simulate the vaporization of isolated *n*-heptane droplets injected into air at 1000 K and at pressures of 1 atm and 10 atm. Their results showed that the spherical droplet initially undergoes strongly damped oscillations and that the circulation within the droplet is the reason for the damping. Their model predicted the vaporization characteristics and the dynamics of the moving droplet quite well.

Suspended droplet evaporation in a laminar convective environment was investigated by Shih and Megaridis[27]. They studied the influence of the suspension fiber on the vaporization characteristics. The influence of the thermal Marangoni effect on droplet evaporation in a convective environment was studied by Shih and Megaridis[28]. In their cases, the thermocapillary effect and vaporization characteristics were independent of the Reynolds number. Tamim and Hallett[29] used a continuous thermodynamics model to describe the mixture composition, properties and vapor–liquid equilibrium. In their model, the composition was represented by a continuous probability density function. The model equations were solved using finite difference method. Dwyer et al.[30] and Dwyer and Shaw[31] used axisymmetric models to investigate surface tension effects on both vaporizing and combusting methanol droplets. Their results indicated that thermal and solutal Marangoni effects can greatly influence the flow patterns within a liquid droplet. The surface tension gradients due to spatial variations of temperature along the interface have a profound impact on droplet dynamic behavior.

Ambient gas solubility: dissolving of ambient gas into the liquid droplet under high pressure conditions.

Aggarwal and Mongia[32] investigated multi-component effects during droplet evaporation at ambient pressures in the range of 1–40 bar using two droplet sub-models. They used surrogate fuel droplet to represent vaporization behavior of a multi-component droplet. Diffusion schemes such as diffusion-limit and infinite-diffusion models were used by them to compare the behavior of multi-component fuel with that of the surrogate fuel. Their model included real gas behavior, solubility of gases in liquid phase and pressure dependent variable thermophysical properties. They investigated the operating conditions under which their assumptions were valid and found that the vaporization characteristics were highly sensitive to the droplet heating models than the blend composition. They attributed this to increase in droplet heat-up time and reduction in volatility differential between constituent fuels at high pressures. Gartung et al.[33] investigated two different droplet vaporization models, discrete and continuous, to describe multi-component vaporization of hydrocarbon blends. Sazhin[34] reviewed and identified unsolved problems in modeling the heating and evaporation of fuel droplets. He concluded that the distillation curve model (DCM) for modeling the evaporation of multi-component droplets seemed to be reasonably accurate and also less expensive. The author used a parabolic method for predicting re-circulation. This, however, was only an approximate method and hence can be used in CFD codes and for applications where accurate calculations are not essential. Yang et al.[35] used a discrete/continuous multi-component model (DCMC) to describe the composition of realistic fuels. Gasoline was assumed to consist of five discrete families of hydrocarbons (*n*-paraffins, *i*-paraffins, naphthenes, aromatics and olefins), each consisting of an infinite number of continuous components, modeled as PDF. They tracked the mean and variance of each PDF. They used an approximate solution to quasi-steady energy equation to derive an explicit expression for heat flux from the gas phase to the gas–liquid interface. They claimed that their procedure resulted in accurate predictions when compared to a continuous multi-component (CMC) model.

Elwardany et al.[36] reported a comparative study of various numerical models, which could predict single-component and multi-component droplet heating and cooling. They considered the effect of moving boundary in their solutions to species diffusion and heat conduction equations. Sazhin et al.[37] developed a simplified numerical model to simulate heating and evaporation in multi-component droplets. Their model took liquid and gas phase coupling into account. They compared the results obtained from their numerical model with the experimental data. Though, the predicted results did not closely match with those from experiments, the prediction was good enough for implementation in CFD codes, where CPU time is an important constraint. Strotos et al.[38] investigated the evaporation behavior of two-component hydrocarbon droplets. They solved the Navier–Stokes equations along with VOF method for tracking the interface, coupled with energy and concentration equations in both liquid and vapor phases.

Marangoni convection: fluid flow induced over a liquid droplet surface as a result of surface tension gradients.

Raghuram et al.[39, 40] and Raghuram and Raghavan[41] numerically studied the transient evaporation of droplets constituted by two fuel components in air at atmospheric pressure, considering suspended as well as moving droplets. They employed a comprehensive two-phase model with variable thermophysical properties and calculated the activity coefficient using UNIFAC group contributions method. The liquid and gas phases were coupled with appropriate interface conditions. They found that solutal Marangoni effect was dominant at low freestream velocity. Tonini and Cossali[42] studied the evaporation of bi-component and tri-component fuel droplets at atmospheric pressure. The surface regression curves for tri-component droplet were quite nonlinear. Azimi et al.[43] numerically studied droplet evaporation of three fuels namely *n*-heptane, decane and hexadecane at ambient temperatures of 500 K and 800 K, and at atmospheric pressure. They reported that the ambient temperature and the type of fuel had significant effects on unsteadiness. Strotos et al.[44] numerically studied the evaporation characteristics of binary hydrocarbon droplets using volume of fluid (VOF) method to track the interface, considering ambient temperatures in the range of 0.56–1.62 times the critical fuel temperature, under atmospheric pressure. They included the effect of suspension fiber in their model. They showed the flow field as the droplet was moving over the suspension fiber. A disadvantage was that their model was reported to be very expensive as their simulations took around 1–3 CPU months.

Some salient findings from few of these models are as follows: based on the fuel volatility, ambient and convective conditions, droplet evaporation has three stages, as shown in Fig. 1.

The volumetric expansion phase may not be predominant for high volatile fuel droplets or at higher ambient temperatures. The strength of forced convection around the evaporating droplet has a significant effect on the Marangoni convection experienced by the droplet. At higher free stream velocities (around 3 m/s) the Marangoni convection becomes weaker and the internal flow field within the droplet is dictated by the forced convective flow. At much lower free stream velocities (less than around 0.3 m/s), it has been observed that the Marangoni convection can induce a flow in the opposite direction to that of the forced convection. In the case of multi-component droplets, at a low relative velocity, multi-cellular vortices, as shown in Fig. 2, are observed within the droplet due to the dominance of solutal Marangoni effects. The evaporation characteristics of binary fuel droplet typically follow the trend shown schematically in Fig. 3.

Here, $z_1 = 0$ corresponds to zero volume fraction of high volatile component and $z_1 = 1$ represents the absence of the low volatility component. It is clear that the volumetric expansion phase is

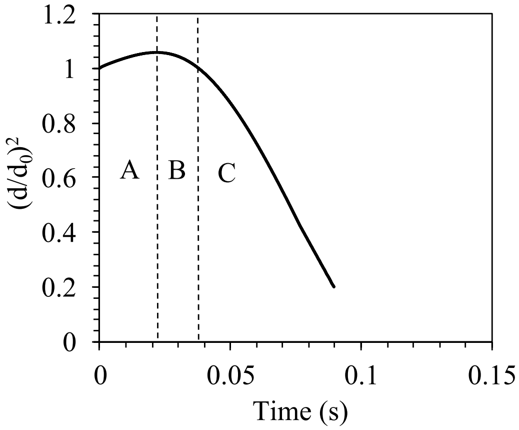

Figure 1: Temporal variation of non-dimensional droplet surface area of a stagnant *n*-dodecane droplet evaporating in oxygen at an ambient temperature of 0.9 time its critical temperature and at its critical pressure, displaying stages such as A: volumetric expansion, B: unsteady evaporation and C: steady evaporation.

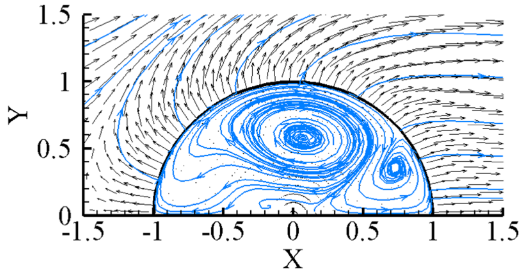

Figure 2: Typical flow field in and around a moving *n*-heptane + *n*-hexadecane droplet (initially 50–50% volume) in nitrogen environment.

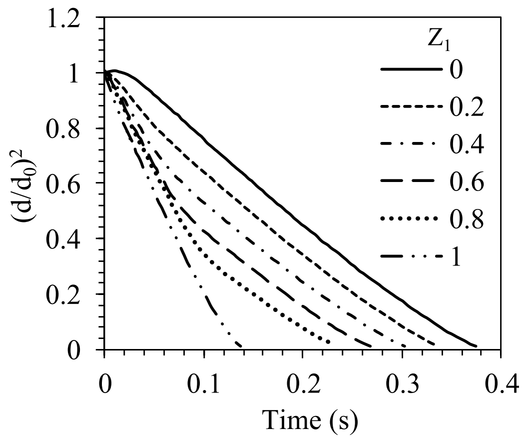

Figure 3: Typical surface regression of a droplet with two-components of distinct volatilities; $z_1 = 0$ corresponds to the presence of only the lower volatility component and $z_1 = 1$ corresponds to the presence of only the higher volatility component.

absent in high volatile droplet evaporation. As the value of z_1 is gradually increased, two distinct slopes are visible. For instance, at $z_1 = 0.6$, for until about 0.1 s, the slope of the droplet regression curve is close to that of high volatile droplet and after that, the slope gradually changes and follows that of low volatility droplet. A definite time period, where the regression curve has an almost constant slope, is also apparent from Fig. 3.

3.2 Numerical Models for Evaporation Under High Ambient Pressures

Even in high-pressure environments, a few of the early investigations assumed steady state, ideal gas behavior of the gas phase, insolubility of ambient gas into liquid phase, and constant properties in both gas and liquid phases. However, these common assumptions that are employed in low-pressure models are not valid at high ambient pressures. At high pressures, the droplet heat-up period and transient behavior of the gas and liquid phases persist throughout the droplet lifetime. At high pressures, even for a single component liquid droplet vaporizing into a single component gas environment, two species are involved in both phases taking into account of vaporization of liquid into vapor-phase and solubility of ambient gas into the liquid phase. Phase equilibrium, in this case, dictated by fugacity balance in liquid and gas phases, is relatively simple, as an algebraic equation results on solving equations involving fugacity coefficients. However, if there are more than one liquid component (or more than one gas in ambient), the phase equilibrium has to be estimated by simultaneously solving the equations involving fugacity coefficients of all these species and a numerical methodology will be required to solve for phase equilibrium.

Studies on droplet evaporation at elevated pressures were mostly limited to stagnant surroundings and only a few studies are reported under convective conditions. Matlosz et al.[45] and Kadota and Hiroyasu[46] experimentally and analytically studied the transient droplet vaporization at high pressures and high temperatures. Both studies employed Redlich–Kwong (RK) equation of state (EOS) to capture the real gas effects. However, the solubility of ambient gas was neglected in their models. Their results indicated that at the higher pressures molecular mass transport may not be the only controlling mechanism for the evaporation process. Manrique and Borman[47], Lazar and Faeth[48] and Canada and Faeth[49] developed theoretical models incorporating RK-EOS, and investigated steady-state vaporization of liquid fuel droplet in sub-critical and super-critical environments. The real gas effects and solubility of nitrogen in liquid fuel were also considered in their models. However, the heat-up of the droplet at high pressures was neglected, which remains important throughout the droplet lifetime. They also pointed that after a sufficient high pressure, steady-state conditions were not attained at all.

Curtis and Farrell[50, 51] developed numerical models, which employed the Peng–Robinson equation of state (PR-EOS), to study of the evaporation of spherical fuel droplets in high-pressure and high-temperature environment. They reported that, if the ambient temperature and pressure were high enough, the droplet may heat up to its critical mixing point in a totally transient manner and coupled diffusion process became important in high-pressure droplet evaporation.

Hsieh et al.[52] presented a comprehensive analysis of high-pressure droplet evaporation for multi-component fuels at a supercritical temperature of 2000 K. Their results showed an increasing trend in the droplet evaporation rate with pressure at the supercritical temperature.

Jia and Gogos[53, 54] also employed PR-EOS to quantify the real gas effects and took into account the liquid phase solubility of ambient gas, for a wide range of ambient pressures and temperatures. Their results showed that at low ambient temperatures, the droplet lifetime presented a maximum with pressure and at high ambient temperatures, it decreased monotonically with pressure. They also reported that with an increasing ambient pressure, the droplet heat-up period increased as a proportion of the droplet lifetime and this became extremely important throughout the entire droplet lifetime for high enough ambient pressures. Delplanque and Sirignano[55] and Haldenwang et al.[56] numerically investigated the transient vaporization of a liquid oxygen droplet in gaseous hydrogen at high pressures. Zhu and Aggarwal[57, 58] numerically investigated the transient vaporization of *n*-heptane droplet in nitrogen environment using different empirical equations of state. Their results showed that the predictions obtained using PR-EOS had an excellent agreement with the experimental data from the literature. At low–moderate ambient temperatures, the droplet lifetime first increased and then decreased as the ambient pressure was increased. However, at high ambient temperatures, the droplet lifetime decreased monotonically with pressure. Gogos et al.[59] pointed out that the droplet lifetime under normal gravity conditions decreased with ambient pressure more significantly than it decreased under microgravity. Consolini et al.[60] reported that at sub-critical conditions, a spherical droplet maintained its spherical shape, while an initially non-spherical droplet attained the spherical shape very early in its lifetime. However, in supercritical environment, the droplet did not maintain the spherical shape and also its temperature increased continuously during the vaporization process. Zhang[61] and Zhang et al.[62] carried out numerical research on a vaporizing n-heptane droplet in a forced convective nitrogen environment at high pressures up to 12 MPa under microgravity. The numerical results showed that at lower ambient pressures, the temperature at the center of the droplet followed the surface temperature faster than the same at higher ambient pressures. It was observed that droplet heating was significant for most of the droplet lifetime, and that at super-critical pressures, the droplet surface temperature reached the computed critical state of the mixture.

Initial conditions and convective effects are extremely important in modeling the transient vaporization process and to arrive at predictions closer to the experimental results. Yang and Wong[63] attempted to explain the discrepancies between theoretical results and available experimental results for microgravity droplet evaporation. They found that, at low ambient temperatures, the discrepancies were mostly due to conduction effects of the fiber, however, the importance of liquid phase radiative absorption increased with increasing temperature. At high ambient pressures (1 MPa and 2 MPa), however, their theoretical results differed substantially from the experimental results of Nomura et al.[64], even with the inclusion of fiber conduction and liquid phase radiation absorption in their model. The enhancement in the droplet evaporation rate due to natural convection was more dominant with increasing ambient pressure. Simulating the cases of Nomura et al.[64], Zhang et al.[65] pointed out that the initial droplet motion from the droplet generation position to the test position was responsible for those discrepancies between numerical predictions and the experimental results of Nomura et al.[64]. Due to relative motion, the droplet experienced a considerable heat-up and the shear stress at the liquid–gas interface introduced a circulation within the droplet interior, which sustained for a quite longer time. They also reported that the final penetration distance of the vaporizing droplet decreased exponentially with ambient pressure. The average evaporation constant increased linearly with pressure for small reduced ambient pressures ($p_r < 2$). However, at high ambient pressures, it either became a constant (for lower initial free stream velocities) or non-linearly increased (at higher initial free stream velocities) with the ambient pressure.

Balaji et al.[66] numerically studied evaporation of stagnant and moving *n*-dodecane droplets in nitrogen environment at high pressures. Their model was also comprehensive enough to include gas phase non-idealities, the liquid phase solubility of gases, and variable thermophysical properties as a function of pressure, temperature and composition. They validated their results against experimental results reported in the literature. Their results indicated that for stagnant droplets, at sub-critical ambient temperatures, droplet lifetime monotonically increased with pressure. At critical temperature, it first increased and remained almost a constant with increasing pressure. At super-critical temperatures, the lifetime decreased continuously with increasing ambient pressure. Here, the average evaporation constant presented a local maximum at the reduced ambient pressure between 2 and 3. For moving droplets, at super-critical ambient temperature, as the initial droplet velocity was increased, the rate of increase of the average evaporation constant with ambient pressure became significant. For low initial droplet velocities (<1 m/s), the average evaporation constant gradually increased with ambient pressure and subsequently became a constant with a further increase in ambient pressure. The droplet lifetime decreased with an increase in ambient pressure and increase of initial droplet velocity. Penetration distance of the moving droplets decreased with ambient pressure and increased with initial droplet velocity. Saroj et al.[67] for the first time reported comprehensive numerical simulations of evaporation of droplets constituted by *n*-heptane and *n*-hexadecane mixtures in high-pressure nitrogen ambient under normal gravity conditions. Gas phase non-idealities, solubility of ambient gas in liquid phase, and pressure and temperature based variable thermophysical properties in both liquid and vapor phases were considered. Phase equilibrium was estimated by an iterative procedure using fugacity coefficients of three species in both phases. The numerical model was validated against the experimental data. Their results showed that, at a given pressure, the droplet lifetime decreased with an increasing ambient temperature. However, at a given ambient temperature, the droplet lifetime first increased with increasing ambient pressure, reached a local maximum and then decreased with a further increase in the ambient pressure. They reported that the initial increasing trend in a lifetime was due to an increase in droplet heat-up period and a decrease in the gas phase mass diffusivity with increasing ambient pressure. However, due to variations in other properties such as surface tension with pressure, at still higher ambient pressures, the evaporation rate increased, resulting in a decreasing trend in the droplet lifetime at these pressures. They further reported that the mass of higher volatility component undergoes a sharp reduction within a short period of lifetime. The ambient gas dissolved into the liquid phase based on the ambient conditions and its mass reached a maximum value at a certain time instant. It then decreased due to net evaporation along with other fuel species. As the freestream velocity was increased, faster evaporation occurred at all pressures. They concluded that the initial composition of the droplet had a significant effect on evaporation at low pressures. On the other hand, at higher pressures, the effects due to initial composition became more and more insignificant. By presenting the fields of velocity, temperature and mass fractions of species, they reported that the gradients of these variables near the droplet surface were quite higher at high pressures than those at lower pressures.

Few studies related to explaining the effects of droplet suspender are also available. Shih and Megaridis[27] and Yang and Wong[68] indicated that liquid fuel evaporation characteristics, the droplet surface regression rates and the droplet surface temperature do not vary appreciably for suspender sizes. However, they concluded that heat conduction through fiber enhances evaporation.

Important observations from these studies are the following: the evaporation constant decreases strongly with ambient pressure for ambient temperature lower than the critical temperature of the fuel. Under microgravity conditions, the evaporation constant is weakly sensitive to pressure for ambient temperatures around the critical temperature of the fuel, however, at substantial super-critical ambient temperatures, the evaporation constant increases with ambient pressure. The evaporation constant under microgravity is smaller than that at the normal gravity. The spherical nature of the droplet is mostly affected in supercritical environment. The effect of suspension fiber was strong when environment temperature was low and when the fiber thickness was large.

The transient effects during the evaporation of an *n*-dodecane droplet in nitrogen ambient at sub-critical, critical and super-critical temperatures of *n*-dodecane are demonstrated in Figs. 4, 5 and 6 considering various values of reduced pressures (ambient pressure divided by critical pressure of the fuel). At ambient temperature close to critical temperature, as the ambient pressure increases, the overall droplet lifetime increases. Volumetric expansion becomes increasingly significant (Fig. 4). Even at critical ambient temperature, the volumetric expansion and droplet lifetime increases as the ambient pressure is increased (Fig. 5). However, at an ambient temperature equal to two times the critical temperature and at a reduced pressure of 6, critical state of mixture (*n*-dodecane and nitrogen) is reached during the evaporation process. Figure 6 illustrates that at ambient conditions of critical pressure and critical temperature of the fuel, a steady evaporation regime appears as indicated

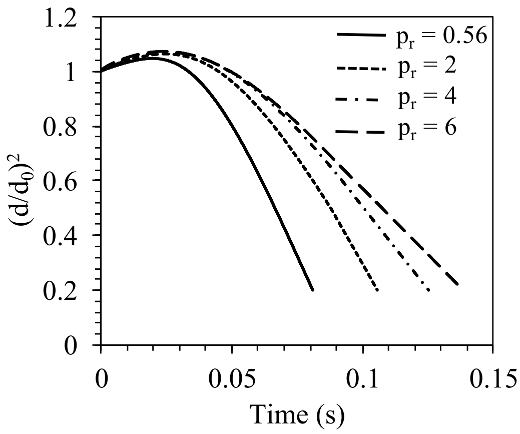

Figure 4: Temporal variation of non-dimensional droplet surface of a stagnant n-dodecane droplet in nitrogen at $T_\infty = 0.9\ T_C$ and different ambient pressures; plotted from data reported in Balaji et al.[66].

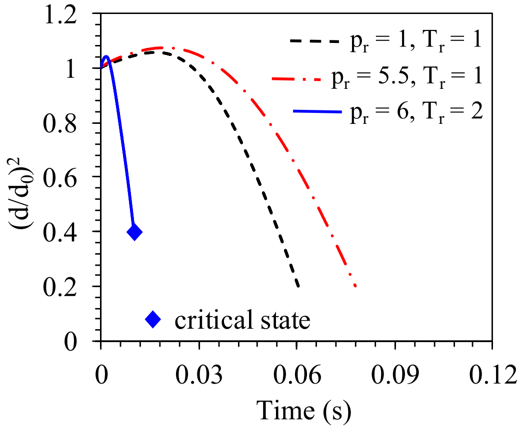

Figure 5: Temporal variation of non-dimensional droplet surface of a stagnant n-dodecane droplet in nitrogen at $T_\infty = T_C$, $p_\infty = p_c$; $T_\infty = T_C$, $p_\infty = 5.5\ p_c$; $T_\infty = 2\ T_C$, $p_\infty = 6\ p_c$; plotted from data reported in Balaji et al.[66].

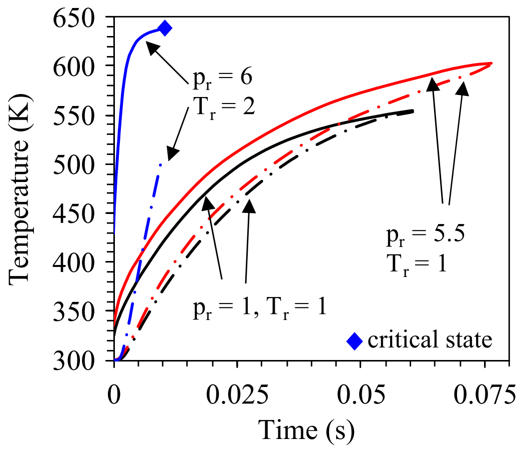

Figure 6: Temporal variation of surface temperature (solid line) and temperature at the droplet center (dashed line) during the evaporation of a stagnant *n*-dodecane droplet in nitrogen at several ambient conditions; plotted from data reported in Balaji et al.[66].

by the merging of surface and center temperatures of the droplet. Even at a reduced pressure of 5.5, droplet center temperature equalizes that of the surface at some time instant. At supercritical ambient conditions ($T_\infty = 2T_C$, $p_\infty = 6p_c$), continued unsteadiness is observed until the droplet reaches the critical state of the mixture.

When a droplet reaches the critical temperature and pressure corresponding to the liquid phase mixture simultaneously, then the interface vanishes, and the liquid and vapor phases cannot be distinguished. If one of the parameter has not reached the critical condition for the mixture, then both liquid and vapor phases continue to exist. For instance, even at a pressure higher than the critical pressure of the mixture, the droplet does not reach critical state, if the droplet temperature is less than critical temperature for the mixture.

4 Numerical Research on Droplet Combustion

Droplet combustion: a liquid fuel droplet burning with a flame zone around its surface.

Numerical models on single droplet combustion have been reported to study phenomena such as flame transition, flame extinction, soot formation and ignition delay, besides other processes. Flame transition occurs due to the relative velocity between the droplet and the surrounding gas. Convective and radiative extinction of flame around the droplet occurs as a result of lower residence time and radiative heat loss, respectively. Soot formation over the droplet surface affects its burning characteristics. When a droplet moves into a hot air environment, based on the ambient temperature and other conditions, a flame is established over its surface. The time delay in the flame formation is one of the spray characteristics. In this section, the literature reporting numerical results on single droplet combustion is presented.

Single step kinetics: representation of the overall reaction between the fuel and oxidizer in one global step.

Steady conservation equations including a single step kinetics for fuel and oxidizer in spherically symmetric coordinates were solved by Polymeropoulos and Peskin[69] to determine the ignition and extinction conditions during the combustion of single fuel droplets. Dwyer and

Sanders[70] presented finite difference solution to steady conservation equations. They were able to predict two distinct flame regimes, namely, envelope and wake flames. Dwyer and Sanders[71] extended their numerical model to include transient effects during the burning of an octane droplet. They were able to predict the movement of wake flame towards the front stagnation point of the droplet to become an envelope flame. Shaw[72] considered liquid phase diffusion to study its influence on spherically symmetric combustion of two-component droplets. Cho et al.[73] employed a transient one-dimensional numerical model with detailed chemical kinetics to predict the characteristics of droplets burning under microgravity environment. They were able to predict the extinction diameter, where the flame around the droplet suddenly vanishes. Chao et al.[74] carried out multi-scale activation energy asymptotic analysis to establish the temperature sensitive nature of radiation heat transfer on the structure and extinction of diffusion flame established over a droplet. They established the dependence of droplet size on radiative extinction. Madooglu and Karagozian[75] developed a model based on boundary layer approach, considering one-step finite rate chemistry and property variation as a function of temperature and composition, to study droplet combustion. Saitoh et al.[76] used a transient model with variable properties and finite rate chemistry to study the effect of thermal radiation on the combustion characteristics of a fuel droplet. It was shown that the inclusion of the radiation model resulted in the reduction of the maximum temperature by around 25%. Huang and Chen[77] investigated the burning characteristics of liquid fuel droplets under forced convection in axisymmetric coordinates using one-step global reaction kinetics. They reported the occurrence of rapid transition of envelope to wake flame under certain air velocity. They also reported that the d^2-law was still valid for droplet combustion in wake flame mode. Jiang et al.[78] reported multiple flame configurations during quasi-steady combustion of fuel droplet using two-phase numerical model and one-step global kinetics. They used Reynolds number and Damköhler number to delineate regimes such as no flame, wake flame and envelope flame. Marchese et al.[79] used transient, bicomponent droplet combustion model to predict the burning features of methanol and methanol–water droplets under microgravity conditions. However, they were not able to predict the non-linearity in the surface regression of the droplets with their model. Marchese and Dryer[80] carried out transient simulations of methanol droplet combustion and concluded that their numerical results were consistent with the experimental results only when internal liquid phase motion was considered by reducing the effective liquid mass Peclet number to an order of one. Lee et al.[81] used spectral element method to model transient droplet combustion in a non-quiescent environment. Detailed kinetics for CO oxidation was used. Huang and Chen[82] modelled the ignition of *n*-heptane droplet in high-temperature convective stream. Both forced convection and gravity-driven natural convection were considered. They reported that an envelope flame forms after ignition and d^2-law was valid in mixed (forced + natural) convective environment as well. Marchese and Dryer[83] and Marchese et al.[84] reported studies on radiative effects on droplet combustion using spherically symmetric transient model and concluded that radiation effects cannot be neglected for droplets with initial droplet diameter more than 3 mm. Dwyer et al.[85] from their numerical simulations of combustion of moving methanol droplets clearly showed that Marangoni convection and diffusion flame interaction exert strong forces on liquid droplets. The liquid phase dynamics are found to be extremely important as indicated by this study. Marangoni convection can induce internal motion within the droplet, which is burning even under quiescent condition, due to factors such as ignition and water absorption. Thus, this parameter is quite important for alcohol droplets, which are polar in nature like water.

Liquid phase motion: fluid flow occurring inside a liquid fuel droplet while it is evaporating.

Balakrishnan et al.[86, 87] reported their porous sphere experiments and related quasi-steady simulations of diffusion (envelope) flames over the droplet (sphere) surface. They used the finite element method. Since such diffusion flames are transport controlled, they used infinite rate chemistry. They formulated their model based on Schvab–Zeldovich method. They were able to predict burning rate of the fuel through the porous sphere as a function of air velocity. They also analyzed the interference between the diffusion flames from two adjacent burning spheres. Kazakov et al.[88] studied ethanol droplet combustion using detailed chemical kinetics and spherically symmetric model. They were able to predict the regression rate as well as extinction diameter. They took into account of water accumulation inside the ethanol droplet using liquid mass Peclet number. Auto-ignition and burning characteristics of isolated fuel droplets were studied using detailed chemical kinetics by Cuoci et al.[89]. They emphasized the influences of radiative heat transfer and low-temperature oxidation mechanisms on the prediction of extinction diameters of *n*-heptane droplets. Studies on *n*-heptane droplet under quiescent and convective environments have been reported by Pope and Gogos[90] and Pope et al.[91]. Using finite volume method, they solved the governing equations in gas phase in an axisymmetric domain. They used one-step global kinetics and were able to predict the air velocity that caused flame extinction. They extended their model to include the solution of liquid phase transport processes and simulated the combustion of moving and suspended droplets. Raghavan et al.[92] conducted porous sphere experiments using methanol and measured the mass burning rate and the air velocity at which envelope flame transitioned to wake flame. They employed an axisymmetric quasi-steady model using one-step kinetics for methanol oxidation and variable thermophysical properties. Their model included the effects of forced and natural convection. They were able to predict the mass burning rates and the air velocity at which a wake flame was obtained. Dietrich et al.[93] conducted microgravity experiments on decane droplet and modelled their experiments using a spherically symmetric transient model with constant properties. They emphasized the importance of fuel vapor accumulation through their transient results. Stauch et al.[94] conducted a detailed numerical simulation of auto-ignition of *n*-heptane droplet burning in hot air. They varied ambient pressure, initial droplet diameter and other initial conditions to study their effects on auto-ignition. The initial droplet size was seen to affect the auto-ignition characteristics more.

Raghavan et al.[95] developed and used an axisymmetric model to predict the extinction diameters of methanol droplet in a quiescent microgravity environment. Their model included variable thermophysical properties calculated as a function of temperature and species concentration, and surface tension gradient term added in the shear stress balance equation at the interface. They used one-step global mechanism for imparting finite-rate chemistry. It was shown that the liquid phase motion was highly responsible for water absorption within the methanol droplet. Solutal and thermal Marangoni effects were able to induce complex, multi-cellular motion within the methanol droplet, which facilitated perfect mixing and realistic water absorption within the droplet. Raghavan et al.[96] predicted the flame characteristics over methanol droplets under forced convection considering both suspended as well as moving droplets. For moving droplets, initially a wake flame appeared and as the droplet decelerated, an envelope flame was formed during some time instant of its life period, for all initial Reynolds number in the range of 1–100. Under this scenario, the surface tension effects were seen to be important for the entire range of Reynolds number. On the other hand, for suspended droplets, the surface tension effects were seen to be important only when Re was less than around 15. Raghavan et al.[97] included optically thin approximation based radiation model in their axisymmetric numerical model and were able to predict the extinction diameters of methanol droplets having an initial diameter in the range of 0.43–3 mm. It was shown that both surface tension and non-luminous thermal radiation were important in predicting the extinction diameter. Raghavan et al.[98] investigated the interference effects during burning of porous spheres kept under tandem arrangement and fueled by methanol. An axisymmetric quasi-steady numerical model was used in the simulations. Both forced as well as natural convection were included. One-step global finite rate kinetics was employed along with variable thermophysical properties. Oxygen starvation and heat flux increment between the flames were found to be the important consequences as a result of interference between the flames over the porous spheres.

Jin and Shaw[99] used a commercial software to study the combustion and extinction of *n*-heptane droplet in air added with carbon-dioxide, helium and xenon. They used VOF method with one-step chemical kinetics and variable thermophysical properties. They reported the importance of Soret effect in predicting droplet combustion characteristics. Sahu and Raghavan[100] presented simulations of steady burning of ethanol over porous spheres using a numerical model that included variable properties, non-luminous thermal radiation and global one-step chemistry. The effect of air velocity on flame behavior was presented in detail. They presented criteria for flame extinction due to forced air flow in terms of Damköhler number and momentum ratio near the front stagnation point of the sphere. Sahu et al.[101] simulated steady burning of spherical ethanol particles in a spray environment, which was modeled as a high-temperature oxidizer stream, where the major products of combustion were present. They reported that the ambient temperature affects the burning rate only when oxygen content in the oxidizer had reduced below a given value. The variation of normalized Damköhler number was presented to delineate the occurrences of combustion and pure evaporation.

Farouk and Dryer[102] simulated tethered methanol droplet combustion in CO_2 environment under microgravity conditions using a spherically symmetric transient numerical model with detailed chemical kinetics. They were able to predict the extinction diameters as well as enhancement in the burning rate, when thick quartz fibers were used. Farouk et al.[103] presented the predictions from their spherically symmetric numerical model along with the results from microgravity experiments on methyl butanoate droplet combustion. Awasthi et al.[104] reported the combustion characteristics of methanol droplet in nearly quiescent and hot environment, and analyzed the effects of initial droplet diameter. The model parameters were almost similar to that of Raghavan et al.[97]. They reported the effects of kinetics, surface tension and radiation for different droplet initial diameters. Awasthi et al.[105] carried out similar investigation on the combustion characteristics of *n*-heptane droplets, where the effects of initial droplet size as well as ambient temperature were revealed.

Cuoci et al.[106] numerically investigated the auto-ignition of isolated *n*-heptane, *n*-decane and *n*-dodecane droplets in air under microgravity conditions, considering pressure in the range of 1–20 bar. They emphasized the importance of low-temperature chemical kinetics from their predictions. Alam et al.[107] and Cheng et al.[108] reported the combustion characteristics of *n*-butanol and butanol isomers. Their transient models included complex combustion chemistry, radiative heat transfer and temperature dependent variable properties. They also made a comparative assessment between two kinetic models. Farouk et al.[109] carried out transient spherically symmetric droplet combustion modeling using detailed chemistry to understand the cool flame burning regime in large diameter droplets under microgravity. Several factors that influenced the dual stage hot flame to cool flame transition or direct establishment of a cool flame were analyzed and discussed. Cuoci et al.[110] employed a detailed mechanism (with 450 species and 17,000 reactions) to simulate low-temperature combustion regime. They were able to predict the experimental results quite well and were able to explain the physics behind low-temperature combustion and flame extinction.

Ashna et al.[111] employed a two-phase lattice-Boltzmann formulation for simulating combustion of *n*-heptane and *n*-butanol droplets. Appropriate source terms were used to account for the heat release from combustion as well as the radiative heat loss. Single step global reaction was considered. Their predictions were validated against the experimental data. Giusti et al.[112, 113] carried out simulations of droplet combustion under gas turbine conditions and high-altitude relight conditions. The effects of increased dilution of product mixture were reported. A regime diagram for droplet evaporation and auto-ignition was presented as a function of initial droplet size and air dilution. In high-altitude conditions, the ignition phenomenon was studied. Stagni et al.[114] used heterogeneous chemical kinetics mechanism, describing aerosol and particle behavior, in their one-dimensional model that accounted for non-luminous and luminous radiative heat losses, to study the soot formation from isolated *n*-heptane droplet flames. Chen et al.[115] reported evaporation and combustion characteristics of liquid hydrogen droplet using one-dimensional (radial coordinate) diffusive equations. They reported about the existence of a critical radius, where the conductive and radiation heat become equal. A front-tracking method was developed for particle-resolved simulations of droplet evaporation and combustion by Irfan and Muradoglu[116]. They used finite-difference front-tracking method to solve the two-phase system. Many benchmark results have been reported in their study. Combustion of *n*-heptane droplet has been simulated using detailed chemical kinetics.

It is clear that several authors have used quasi-steady models to predict the steady burning characteristics of liquid fuels. Here, the liquid phase transport processes are not included. Gas phase simulations are made as comprehensive as required. These studies mimic the conditions of porous sphere experiments, where the liquid fuel is supplied to the porous sphere uniformly at the rate at which it burns. Burning rates, convective extinction and transition of envelope to wake flames under different ambient conditions were reported in these studies. Figure 7 presents the variation of predicted mass burning rates as a function of air velocity for different sizes of porous spheres. The quasi-steady model is able to predict the increasing trends in the mass burning rate with an increase in air velocity as well as the sphere diameter.

Several researchers have used spherically symmetric droplet combustion model to predict the combustion characteristics under microgravity conditions. All comprehensive features such as time dependency, variable thermophysical properties, radiation sub-model and detailed chemical kinetics have been considered in many of these models. They were able to predict the droplet burning characteristics under micro-gravity environment when fuel oils such as *n*-heptane, *n*-decane and *n*-dodecane were employed. However, when combustion of alcohol droplets, especially the methanol droplet, was simulated, liquid phase transport becomes quite important. At least an axisymmetric model was required for predictive simulation alcohol droplet combustion. Here, the inclusion of surface tension effects triggers Marangoni convection. For such a comprehensive axisymmetric model that includes two-phase time-dependent transport, variable thermophysical properties, multi-component diffusion including the Soret effect and radiation sub-model, several researchers restricted their kinetics model to global single step reaction. Apart from droplet surface regression, transition from wake to envelope flame and vice versa, flame extinction due to convection and radiation, and auto-ignition of droplets under hot ambient conditions were predicted close to experiments. Table 1 presents the extinction diameters of methanol droplet as predicted by a model that neglects surface tension and flame radiation, a model that includes surface tension, but neglects flame radiation and the model that includes both. It is clear that the model that includes both the effects is able to predict higher extinction diameter, comparable to the reported experimental results.

For moving droplets with initial Reynolds numbers greater than 10, an envelope flame is not readily formed over the droplet surface and the moving droplet must decelerate sufficiently before an envelope flame is formed. The evaporation constant sharply increases after the envelope flame is formed. Figure 8 presents the variation of droplet lifetime and time for which an envelope flame is present over a moving methanol droplet at different initial Reynolds numbers (Raghavan et al.[96]). When the initial Re is increased from 10 to approximately 30, the droplet lifetime increases and time for which an envelope flame is present decreases sharply. When initial Re is increased beyond 30, the droplet lifetime remains almost a constant and the time for which an envelope flame is present decreases gradually. Flame extinction due to water absorption occurs for moving methanol droplets, and this is predicted only when surface tension effects are included.

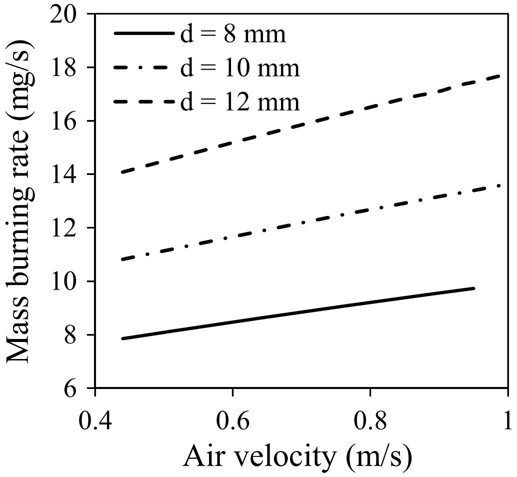

Figure 7: Variation of predicted mass burning rates of porous spheres fueled by ethanol (plotted from data reported in Sahu and Raghavan[100]).

Table 1: Effects of surface tension and non-luminous radiation on extinction diameters of methanol droplet burning under microgravity conditions; case 1 is without surface tension and radiation sub-model, case 2 is with surface tension but without radiation sub-model and case 3 is with surface tension and radiation sub-model (data from Raghavan et al.[97]).

	Extinction diameter (microns)		
Initial diameter (microns)	Case 1	Case 2	Case 3
430	74.85	120.17	130
860	86.85	214.3	228
1720	174	376.05	505
2200	–	476	701
3000	–	661	1123

Few studies report the usage of techniques such as VOF method and lattice Boltzmann method to simulate droplet combustion. Few studies report simulation of isolated droplet combustion in gas turbine and high-altitude conditions. Soot formation in droplet combustion has also been modeled.

5 Summary

In this review, numerical models employed for simulating evaporation and combustion processes of isolated liquid fuel droplets have been presented. A general numerical formulation detailing the conservation of mass, momentum, species and energy in gas and liquid phases, along with interface coupling conditions has been presented.

Numerical models for isolated droplet evaporation are categorized as models for

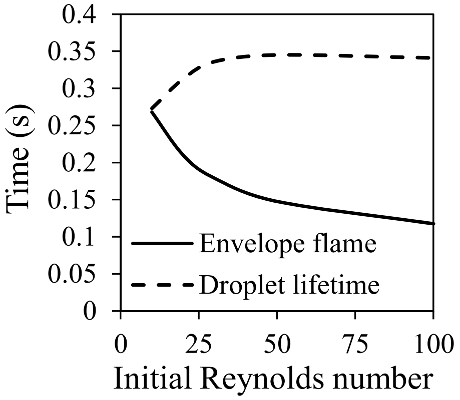

Figure 8: Variations of droplet lifetime and the time for which an envelope flame is present over a moving methanol droplet as a function of initial Reynolds number; plotted from data reported in Raghavan et al.[96].

low–moderate pressures and those for high pressures. In the former, ideal gas equation of state is generally valid and in the latter, a real gas equation of state is employed. A comprehensive model includes temperature and pressure dependent evaluation of thermophysical properties for each species, an appropriate mixing rule to arrive at the mixture properties at a given temperature, pressure and composition, and multi-component diffusion. Under high pressures, the ambient gas dissolves into the liquid droplet. This effect has to be added in the numerical model. Most of the reported works assume that the droplet remains spherical during its evaporation and have validated their predictions against experimental results available under several ambient and convective conditions. Numerical models employing interface tracking schemes such as VOF method, are also available in the literature. Numerical models simulating the evaporation process of multi-component fuel droplet are also reviewed. Liquid phase transport becomes quite important in these simulations. Complex recirculation patterns within the vaporizing droplet have been revealed by the researchers. The models used for predicting these features include surface tension effects to induce Marangoni convection. Preferential vaporization of higher volatile component has been predicted. In the case of multi-component droplet evaporation under high-pressure conditions, the phase equilibrium, which is governed by equating fugacity of each species in liquid and gas phases, has to be solved iteratively.

Numerical models for isolated droplet combustion include quasi-steady and transient models. Quasi-steady models are often used to simulate the steady burning behavior of droplets and liquid fuel fed porous spheres. Here, the gas phase is solved in a comprehensive manner along with interface coupling conditions. Liquid phase is not solved. Axisymmetric models are commonly employed in these. There are several models that use constant properties (calculated at an average temperature) and many others use variable properties. Most of these models use global single step reaction for implementing finite rate kinetics and a few those simulate diffusion flames around the liquid fuel particles, use infinite rate chemistry. The main purpose of these models is to predict the mass burning rate, flame transition from envelope to wake flame and convective extinction.

Transient numerical models for droplet combustion have been used to predict extinction diameter, which is the instantaneous diameter when the flame around a fuel droplet extinguishes under quiescent microgravity conditions. Several authors have used one-dimensional (spherically symmetric) model along with detailed chemical kinetics mechanism. An appropriate radiation sub-model has also been employed by several authors. Many others, who have used the axisymmetric model to simulated droplet combustion under quiescent microgravity conditions, have used global single-step kinetics. However, in these axisymmetric models, liquid phase transport model is quite comprehensive and includes surface tension effects. Combustion in a forced convective environment of suspended and moving droplets can be simulated using axisymmetric model. Combustion in a mixed convective (forced and natural convection) condition can be simulated using the axisymmetric model when the relative gas flow is aligned to the gravity induced flow. Auto-ignition of the droplet in hot gas environment has also been reported by several authors. Ignition and extinction can be predicted only when finite rate chemistry is employed in the gas phase. Several authors have simulated alcohol droplet combustion quite comprehensively. The droplet flame extinction and the complex liquid phase motion are revealed in detail when water absorption into the droplet is modelled accurately by including Marangoni convection in an axisymmetric model.

Authors have revealed a cool flame phenomenon during droplet combustion. The effects of the presence of gases of combustion and flight conditions have also been studied by a few. Some have studied soot formation during droplet combustion. Few studies report the usage of techniques such as VOF method and lattice Boltzmann method to simulate droplet combustion.

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References

1. Williams A (1973) Combustion of droplet of liquid fuels: a review. Combust Flame 21:1–31
2. Faeth GM (1977) Current status of droplet and liquid combustion. Prog Energy Combust Sci 3:191–224
3. Law CK (1982) Recent advances in droplet vaporization and combustion. Prog Energy Combust Sci 8:171–201
4. Faeth GM (1983) Evaporation and combustion of sprays. Prog Energy Combust Sci 9:1–76
5. Sirignano WA (1983) Fuel droplet vaporization and spray combustion theory. Prog Energy Combust Sci 9:291–322
6. Dwyer HA (1989) Calculations of droplet dynamics in high temperature environment. Prog Energy Combust Sci 15:131–158
7. Law CK, Faeth GM (1994) Opportunities and challenges of combustion in microgravity. Prog Energy Combust Sci 20:65–113
8. Gilver SD, Abraham J (1996) Supercritical droplet vaporization and combustion studies. Prog Energy Combust Sci 22:1–28
9. Biroul M, Gökalp I (2006) Current status of droplet evaporation in turbulent flows. Prog Energy Combust Sci 32:408–423
10. Tong AY, Sirognanao WA (1986) Multicomponent droplet vaporization in a high temperature gas. Combust Flame 66:221–235
11. Gogos G, Ayyaswamy PS (1988) A model for the evaporation of a slowly moving droplet. Combust Flame 74:111–129
12. Aharon I, Shaw BD (1996) Marangoni instability of bi-component droplet gasification. Phys Fluids 8:1820–1827
13. Ha VM, Lai CL (2002) Onset of Marangoni instability of a two-component evaporating droplet. Int J Heat Mass Transf 45:5143–5158
14. Ha VM, Lai CL (2004) Theoretical analysis of Marangoni instability of an evaporating droplet by energy method. Int J Heat Mass Transf 45:5143–5158
15. Ra Y, Reitz RD (2003) The application of a multicomponent droplet vaporization model to gasoline direct injection engines. Int J Engine Res 4:193–218
16. Tonini S, Cossali GE (2012) An analytical model of liquid drop evaporation in gaseous environment. Int J Ther Sci 57:45–53
17. Law CK (1978) Internal boiling and superheating in vaporizing multicomponent droplets. Am Inst Chem Eng J 24:626–632
18. Abramzon B, Sirignanao W (1989) Droplet vaporization model for spray combustion calculations. Int J Heat Mass Transf 32:1605–1618
19. Haywood RJ, Nafziger R, Renksizbulut MA (1989) A detailed examination of gas and liquid phase transient processes in convective droplet evaporation. J Heat Transf 111:495–502
20. Megaridis CM, Sirignano WA (1990) Numerical modeling of a vaporizing multicomponent droplet. Proc Combust Inst 23:1413–1421
21. Megaridis CM, Sirignano WA (1993) Multicomponent droplet vaporization in a laminar convective environment. Combust Sci Technol 87:27–44
22. Chiang CH, Raju MS, Sirignano WA (1992) Numerical analysis of convecting, vaporizing fuel droplet with variable properties. Int J Heat Mass Transf 35:1307–1324
23. Megaridis CM (1993) Liquid phase variable property effects in multicomponent droplet convective evaporation. Combust Sci Technol 92:293–311
24. Megaridis CM (1993) Comparison between experimental measurements and numerical predictions of internal temperature distributions of a droplet vaporizing under high convective conditions. Combust Flame 93:287–302
25. Renksizbulut M, Bussmann M (1993) Multicomponent droplet evaporation at intermediate Reynolds numbers. Int J Heat Mass Transf 36:2827–2835
26. Haywood RJ, Renksizbulut M, Raithby GD (1994) Transient deformation and evaporation of droplets at intermediate Reynolds numbers. Int J Heat Mass Transf 37:1401–1409
27. Shih AT, Megaridis CM (1995) Suspended droplet evaporation modeling in a laminar convective environment. Combust Flame 102:256–270
28. Shih AT, Megaridis CM (1996) Thermocapillary flow effects on convective droplet evaporation. Int J Heat Mass Transf 39:247–257
29. Tamim J, Hallet WLH (1995) A continuous thermodynamics model for multicomponent droplet vaporization. Chem Eng Sci 50:2933–2942
30. Dwyer HA, Aharon I, Shaw BD, Niazmand H (1996) Surface tension influences on methanol droplet vaporization in the presence of water. Proc Combust Inst 26:1613–1619
31. Dwyer HA, Shaw BD (2001) Marangoni and stability studies on fiber-supported methanol droplets evaporating in reduced gravity. Combust Sci Technol 162:331–346
32. Aggarwal SK, Mongia HC (2002) Multicomponent and high-pressure effects on droplet vaporization. J Eng Gas Turbines Power 124:248–255
33. Gartung K, Arndt S, Seibel C (2002) Vaporization of multicomponent fuel droplets: numerical and experimental examination. In: Proc. of 18nd annual conference on liquid atomization and spray systems (Europe), Zaragoza, Spain, September 9–11

34. Sazhin SS (2006) Advanced models of fuel droplet heating and evaporation. Prog Energy Combust Sci 32:162–214
35. Yang S, Ra Y, Reitz RD (2010) A vaporization model for realistic multicomponent fuels. In: Proc. of 22nd annual conference on liquid atomization and spray systems (USA), Cincinnati, OH, May 16–19
36. Elwardany AE, Gusev IG, Castanet G, Lemoine F, Sazhin SS (2011) Mono- and multicomponent droplet cooling/heating and evaporation: comparative analysis of numerical models. Atom Sprays 21:907–931
37. Sazhin SS, Elwardany AE, Krutitskii PA, Depredurand V, Castanet G, Lemoine F, Sazhina EM, Heikal MR (2011) Multi-component droplet heating and evaporation: numerical simulation versus experimental data. Int J Therm Sci 50:1164–1180
38. Strotos G, Gavaises M, Theodorakakos A, Bergeles G (2011) Numerical investigation of the evaporation of two-component droplets. Fuel 90:1492–1507
39. Raghuram S, Raghavan V (2012) Numerical study of transient evaporation of moving two-component fuel droplets. At Sprays 22:493–513
40. Raghuram S, Raghavan V, Pope DN, Gogos G (2012) Numerical study of Marangoni convection during transient evaporation of two-component droplet under forced convective environment. Int J Heat Mass Transf 55:7949–7957
41. Raghuram S, Raghavan V, Pope DN, Gogos G (2013) Two-phase modeling of evaporation characteristics of blended methanol-ethanol droplets. Int J Multiph Flow 52:46–59
42. Tonini S, Cossali GE (2015) A novel formulation of multi-component drop evaporation models for spray applications. Int J Therm Sci 89:245–253
43. Azimi A, Arabkhalaj A, Ghassemi H, Markadeh RS (2017) Effects of unsteadiness on droplet evaporation. Int J Ther Sci 120:354–365
44. Strotos G, Malgarinos I, Nikolopoulos N, Gavaises M (2016) Predicting the evaporation rate of stationary droplets with the VOF methodology for a wide range of ambient temperature conditions. Int J Therm Sci 109:253–262
45. Matlosz RL, Leipziger S, Torda TP (1972) Investigation of liquid droplet evaporation in a high temperature and high pressure environment. Int J Heat Mass Transf 15:831–852
46. Kadota T, Hiroyasu H (1976) Evaporation of a single droplet at elevated pressures and temperatures. Bull JSME 19:1515–1521
47. Manrique JA, Borman GL (1969) Calculations of steady state droplet vaporization at high ambient pressure. Int J Heat Mass Transf 12:1081–1095
48. Lazar RS, Faeth GM (1971) Bipropellant droplet combustion in the vicinity of the critical point. Proc Combust Inst 13:743–753
49. Canada GS, Faeth GM (1973) Fuel droplet burning rates at high pressures. Proc Combust Inst 14:1345–1354
50. Curtis EW, Farrell PV (1988) Droplet vaporization in a super critical microgravity environment. Acta Astronaut 17:1189–1193
51. Curtis EW, Farrell PV (1992) A numerical study of high-pressure droplet vaporization. Combust Flame 90:85–102
52. Hsieh KC, Shuen JS, Yang V (1991) Droplet vaporization in high-pressure environments I: near critical conditions. Combust Sci Technol 76:111–132
53. Jia H, Gogos G (1992) Investigation of liquid droplet evaporation in sub-critical and super-critical gaseous environments. J Thermophys Heat Transf 6:738–745
54. Jia H, Gogos G (1993) High pressure droplet vaporization; effects of liquid phase gas solubility. Int J Heat Mass Transf 36:4419–4431
55. Delplanque JP, Sirignano WA (1993) Numerical study of the transient vaporization of an oxygen droplet at sub-critical and super-critical conditions. Int J Heat Mass Transf 36:303–314
56. Haldenwang P, Nicoli C, Daou J (1996) High pressure vaporization of LOX droplet crossing the critical conditions. Int J Heat Mass Transf 39:3453–3464
57. Zhu GS, Aggarwal SK (2000) Droplet super-critical vaporization with emphasis on equation of state. Int J Heat Mass Transf 43:1157–1171
58. Zhu GS, Aggarwal SK (2002) Fuel droplet evaporation in a super-critical environment. ASME J Eng Gas Turbines Power 124:762–770
59. Gogos G, Soh S, Pope DN (2003) Effects of gravity and ambient pressure on liquid fuel droplet evaporation. Int J Heat Mass Transf 46:283–296
60. Consolini L, Aggarwal SK, Murad S (2003) A molecular dynamics simulation of droplet evaporation. Int J Heat Mass Transf 46:3179–3188
61. Zhang H (2004) Numerical research on a vaporizing fuel droplet in a forced convective environment. Int J Multiph Flow 30(2):181–198
62. Zhang H, Raghavan V, Gogos G (2008) Subcritical and supercritical droplet evaporation within a zero gravity environment: low Weber number relative motion. Int Commun Heat Mass Transf 35:385–394
63. Yang JR, Wong SC (2001) On the discrepancies between theoretical and experimental results for microgravity droplet evaporation. Int J Heat Mass Transf 44:4433–4443
64. Nomura H, Ujiie Y, Rath HJ, Sato J, Kono M (1996) Experimental study of high-pressure droplet evaporation using microgravity conditions. In: Proc. 26th Symp. on combustion, The Combustion Institute, Pittsburgh, PA, 1267–1273
65. Zhang H, Raghavan V, Gogos G (2009) Subcritical and supercritical droplet evaporation within a zero gravity environment; on the discrepancies between theoretical

and experimental results. Int J Spray Combust Dyn 1:317–338

66. Balaji B, Raghavan V, Ramamurthi K, Gogos G (2011) A numerical study of evaporation characteristics of spherical *n*-dodecane droplets in high pressure nitrogen environment. Phys Fluids 23(6):063601
67. Saroj R, Raghavan V, Gogos G (2018) Two-phase transient simulations of evaporation characteristics of two-component liquid fuel droplets at high pressures. Int J Multiph Flow. https://doi.org/10.1016/j.ijmultiphaseflow.2018.10.002
68. Yang JR, Wong SC (2002) An experimental and theoretical study of the effects of heat conduction through the support fiber on the evaporation of a droplet in a weakly convective flow. Int J Heat Mass Transf 45:4589–4598
69. Polymeropoulos CE, Peskin RL (1969) Ignition and extinction of liquid fuel drops—numerical computations. Combust Flame 13:166–172
70. Dwyer HA, Sanders BR (1986) A detailed study of burning fuel droplets. In: Symposium (international) on combustion. 21, 633–639
71. Dwyer HA, Sanders BR (1988) Calculations of unsteady reacting droplet flows. In: Symposium (international) on combustion. 22, 1923–1929
72. Shaw BD (1990) Studies of influences of liquid phase species diffusion on spherically symmetric combustion of miscible binary droplets. Combust Flame 81:277–288
73. Cho SY, Choi MY, Dryer FL (1991) Extinction of a free methanol droplet in microgravity. In: Symposium (international) on combustion, 23, 1611–1617
74. Chao BH, Law CK, T'ien JS (1991) Structure and extinction of diffusion flames with flame radiation. In: Symposium (international) on combustion, 23, 523–531
75. Madooglu K, Karagozian AR (1993) Burning of a spherical fuel droplet in a uniform flow field with exact property variation. Combust Flame 94:321–329
76. Saitoh T, Yamazaki K, Viskanta R (1993) Effect of thermal radiation on transient combustion of a fuel droplet. AIAA J Thermophys Heat Trans 7:94–100
77. Huang LW, Chen CH (1995) Flame stabilization and blow off over a single droplet. Numer Heat Transf A 27:53–71
78. Jiang TL, Chen WS, Tsai MJ, Chiu HH (1995) A numerical investigation of multiple flame configurations in convective droplet gasification. Combust Flame 103:221–238
79. Marchese AJ, Dryer FL, Colantonio RO, Nayagam V (1996) Microgravity combustion of methanol and methanol/water droplets: drop tower experiments and model predictions. In: Symposium (international) on combustion, 26, 1209–1217
80. Marchese AJ, Dryer FL (1996) The effect of liquid mass transport on the combustion and extinction of bicomponent droplets of methanol and water. Combust Flame 105:104–122
81. Lee J, Tomboulides AG, Orszag SA, Yetter RA, Dryer FL (1996) A transient two-dimensional chemically reactive flow model: fuel particle combustion in a nonquiescent environment. In: Symposium (international) on combustion, 26, 3059–3065
82. Huang LW, Chen CH (1997) Droplet ignition in a high-temperature convective environment. Combust Flame 109:145–162
83. Marchese AJ, Dryer FL (1997) The effect of non-luminous thermal radiation in microgravity droplet combustion. Combust Sci Technol 124:371–402
84. Marchese AJ, Dryer FL, Colantonio RO (1998) Radiative effects in space-based methanol-water droplet combustion experiments. Proc Combust Inst 27:2627–2634
85. Dwyer HA, Shaw BD, Niazmand H (1998) Droplet/flame interactions including surface tension influences. In: Symposium (international) on combustion, 27, 1951–1957
86. Balakrishnan P, Sundararajan T, Natarajan R (2000) Interference effects during burning of tandem porous spheres in mixed convective environment. AIAA J 38:1889–1898
87. Balakrishnan P, Sundararajan T, Natarajan R (2001) Combustion of a fuel droplet in a mixed convective environment. Combust Sci Tech 163:77–106
88. Kazakov A, Conley J, Dryer FL (2003) Detailed modeling of an isolated, ethanol droplet combustion under microgravity conditions. Combust Flame 134:301–314
89. Cuoci A, Mehl M, Buzzi-Ferraris G, Faravelli T, Manca D, Ranzi E (2005) Autoignition and burning rates of fuel droplets under microgravity. Combust Flame 143:211–226
90. Pope DN, Gogos G (2005) Numerical simulation of fuel droplet extinction due to forced convection. Combust Flame 142:89–106
91. Pope DN, Howard D, Lu K, Gogos G (2005) Combustion of moving droplets and suspended droplets: transient numerical results. J Thermophys Heat Transf 19:273–281
92. Raghavan V, Babu V, Sundararajan T, Natarajan R (2005) Flame shapes and burning rates of spherical fuel particles in a mixed convective environment. Int J Heat Mass Transf 48:5354–5370
93. Dietrich DL, Struk PM, Ikegami M, Xu G (2005) Single droplet combustion of decane in microgravity: experiments and numerical modelling. Combust Theor Model 9:569–585
94. Stauch R, Lipp S, Maas U, Rudman M (2006) Detailed numerical simulations of the autoignition of single *n*-heptane droplets in air. Combust Flame 145:533–542
95. Raghavan V, Pope DN, Howard D, Gogos G (2006) Surface tension effects during low-Reynolds-number methanol droplet combustion. Combust Flame 145:791–807

96. Raghavan V, Pope DN, Gogos G (2006) Effects of forced convection and surface tension during methanol droplet combustion. J Thermophys Heat Transf 20:787–798
97. Raghavan V, Pope DN, Gogos G (2008) Effect of non-luminous flame radiation during methanol droplet combustion. Combust Sci Technol 180:546–564
98. Raghavan V, Babu V, Sundararajan T (2009) Investigation of interaction between methanol fed tandem porous spheres burning in a mixed convective environment. Combust Theor Model 13:461–485
99. Jin Y, Shaw BD (2010) Computational modeling of *n*-heptane droplet combustion in air–diluent environments under reduced-gravity. Int J Heat Mass Transf 53:5782–5791
100. Sahu VK, Raghavan V (2011) A numerical study of steady diffusion flames established over ethanol fed porous spheres. Arch Combust 31:211–222
101. Sahu VK, Raghavan V, Pope DN, Gogos G (2011) Numerical modeling of steady burning characteristics of spherical ethanol particles in a spray environment. J Heat Transf 133:094502
102. Farouk T, Dryer FL (2012) Tethered methanol droplet combustion in carbon-dioxide enriched environment under microgravity conditions. Combust Flame 159:200–209
103. Farouk TI, Liu YC, Savas AJ, Avedisian CT, Dryer FL (2013) Sub-millimeter sized methyl butanoate droplet combustion: microgravity experiments and detailed numerical modeling. Proc Combust Inst 34:1609–1616
104. Awasthi I, Gogos G, Sundararajan T (2013) Effects of size on combustion of isolated methanol droplets. Combust Flame 160:1789–1802
105. Awasthi I, Pope DN, Gogos G (2014) Effects of the ambient temperature and initial diameter in droplet combustion. Combust Flame 161:1883–1899
106. Cuoci A, Frassoldati A, Faravelli T, Ranzi E (2015) Numerical modeling of auto-ignition of isolated fuel droplets in microgravity. Proc Combust Inst 35:1621–1627
107. Alam FE, Liu YC, Avedisian CT, Dryer FL, Farouk TI (2015) n-Butanol droplet combustion: numerical modeling and reduced gravity experiments. Proc Combust Inst 35:1693–1700
108. Cheng LY, Alam FE, Yuhao X, Dryer FL, Avedisian CT, Farouk TI (2016) Combustion characteristics of butanol isomers in multiphase droplet configurations. Combust Flame 169:216–228
109. Farouk TI, Dietrich D, Alam FE, Dryer FL (2017) Isolated *n*-decane droplet combustion—dual stage and single stage transition to “Cool Flame” droplet burning. Proc Combust Inst 36:2523–2530
110. Cuoci A, Saufi AE, Frassoldati A, Dietrich DL, Williams FA, Faravelli T (2017) Flame extinction and low-temperature combustion of isolated fuel droplets of *n*-alkanes. Proc Combust Inst 36:2531–2539
111. Ashna M, Rahimian MH, Fakhari A (2017) Extended lattice Boltzmann scheme for droplet combustion. Phys Rev E 95:053301
112. Giusti A, Sidey JAM, Borghesi G, Mastorakos E (2017) Simulations of droplet combustion under gas turbine conditions. Combust Flame 184:101–116
113. Giusti A, Sitte MP, Borghesi G, Mastorakos E (2018) Numerical investigation of kerosene single droplet ignition at high-altitude relight conditions. Fuel 225:663–670
114. Stagni A, Cuoci A, Frassoldati A, Ranzi E, Faravelli T (2018) Numerical investigation of soot formation from microgravity droplet combustion using heterogeneous chemistry. Combust Flame 189:393–406
115. Chen W, Gao R, Sun J, Lei Y, Fan X (2018) Modeling of an isolated liquid hydrogen droplet evaporation and combustion. Cryogenics 96:151–158
116. Irfan M, Muradoglu M (2018) A front tracking method for particle resolved simulation of vaporization and combustion of a fuel droplet. Comput Fluids 174:283–299

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