Modeling Near Critical and Supercritical Fuel Injection and Mixing in Gas Turbine Applications

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| Citation       | Lettieri, Claudio et al. “Modeling Near Critical and Supercritical Fuel Injection and Mixing in Gas Turbine Applications.” Proceedings of ASME Turbo Expo 2018: Turbomachinery Technical Conference and Exposition, June 11-15, 2018, Oslo, Norway. American Society of Mechanical Engineers, 2018. |
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| As Published   | http://dx.doi.org/10.1115/gt2018-75195                                                                                                                                                            |
| Publisher      | American Society of Mechanical Engineers                                                                                                                                                          |
| Version        | Final published version                                                                                                                                                                            |
| Citable link   | https://hdl.handle.net/1721.1/123675                                                                                                                                                              |
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ABSTRACT
This paper presents a numerical framework for characterizing fuel injection in modern combustors. The approach utilizes scaling analysis to describe the droplet evaporation in non-dimensional and fluid-independent terms. The results of the model are validated against published experimental data of isolated droplets evaporating at subcritical and near-critical conditions. The model is incorporated in a spray calculation framework and extended to the supercritical regime to assess the impact of different fluid-properties and evaporation models on temperature and fuel vapor distributions.

The results suggest that in a non-convective environment the transient and quasi-steady evaporation rates vary exponentially with Lewis number. Furthermore, the results show fluid-independent behavior of the droplet evaporation, indicating that a single-component fluid can potentially be used as a modeling surrogate for jet fuel. The first-principles analysis demonstrates that classical evaporation models overestimate transient evaporation and underestimate quasi-steady evaporation, with discrepancies up to 70% at supercritical conditions. This is due to limitations in fuel-property description and the lack of non-isothermal droplet characterization at near-critical conditions. The temperature profiles are typically under-predicted and fuel vapor concentrations are over-predicted in standard spray calculations with subcritical evaporation models. As such the proposed framework breaks new ground in modeling of supercritical fuel injection. The improved quality in the predicted fuel concentration and temperature distribution can enable more accurate assessment of flame position, improving the estimation of combustion stability margins and NOx emissions. The model can be incorporated in commercial codes to guide the design of combustors operating at supercritical conditions.

NOMENCLATURE

| Symbol | Description |
|--------|-------------|
| Bi     | Biot number, $Bi = h_{conv}d/\lambda_t$ |
| d      | Droplet diameter, [m] |
| D      | Mass-diffusion coefficient, $[m^2/s]$ |
| Fo     | Fourier number, $Fo = \alpha t_e/R^2$ |
| h_{conv} | Convective heat transfer coefficient $[kg \cdot s^{-3} \cdot K^{-1}]$ |
| K_ev   | Evaporation rate $[m^2/s]$, $d(d^2/dt^2)/d(t/d^2_t)$ |
| K'_ev  | Non-dimensional $K_{ev}$, $K'_ev = K_{ev}/\alpha m b$ |
| Le     | Lewis number, $Le = \alpha /D$ |
| p      | Pressure $[Pa]$ |
| Pe_m   | Peclet mass transfer number, $Pe_m = uR/D$ |
| Pe_th  | Peclet thermal transfer number, $Pe_th = uR/\alpha$ |
| R      | Droplet radius $[m]$ |
| t      | Time $[s]$ |
| t_adv  | Characteristic advection time scale $[s]$ |
| t_e    | Evaporation time $[s]$ |
| t_h    | Heating time $[s]$ |
| t_m    | Characteristic mass-diffusion time scale $[s]$ |
| T      | Temperature $[K]$ |
| u      | Velocity $[m/s]$ |
| x      | Axial coordinate $[m]$ |

Greek symbols

| Symbol | Description |
|--------|-------------|
| \(\alpha\) | Thermal diffusivity $[m^2/s]$ |
| \(\lambda\) | Thermal conductivity $[kg \cdot m^{-1} \cdot s^{-3} \cdot K^{-1}]$ |

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\[ \rho \quad \text{Density [kg/m}^3\text{]} \]
\[ \sigma \quad \text{Surface tension [kg/s}^2\text{]} \]
\[ \omega \quad \text{Reduced frequency,} \]

**Subscripts/superscripts**

* Non-dimensional
0 Initial value
amb/AG Ambient value/Ambient gas
c Critical value
g Gas
l Liquid
r Reduced value (normalized by critical value)
v Vapor

1. **INTRODUCTION**

Combustion of fossil fuels in transportation and power generation systems accounts for 70% of emissions worldwide. Aviation-related emissions account for about 3% of the total greenhouse gas emissions in the US alone [1]. The average number of passengers has grown by 5% per year and without a strong innovation impulse, aviation emissions will rise by 42% in 2020 [2]. Levels of pollutants associated with aviation have steadily declined, but nitrous oxide (NO\textsubscript{x}) emissions have been the most challenging to control. Increasingly stringent NO\textsubscript{x} regulations impose severe limitations on the development of fuel-efficient gas turbine engines. On the one hand engine propulsion efficiency increases with turbine inlet temperature, on the other hand NO\textsubscript{x} emissions rise dramatically at high temperatures. The so-called thermal NO\textsubscript{x} is formed in the hot, fuel rich regions near evaporating droplets caused by incomplete atomization and poor mixing. At pressure and temperature above the critical value, the classic distinction between gas and liquid disappears and fluids become supercritical. The supercritical state is characterized by a gas-like diffusive behavior that promotes the rapid mixing of the fuel with the ambient air. This has the potential to decrease the maximum flame temperature, reducing the formation of pollutants and yielding cleaner burning [3].

Recent developments in manufacturing and material technologies have enabled combustors operating at conditions above the critical pressure and temperature of most fuels. The majority of fuels reach supercritical conditions for pressures in the range of about 15-30 atm. For instance, the critical temperature and pressure of Jet A fuel are 398°C and 23.5 bar respectively. In comparison, the pressure ratio of gas turbines has been increasing at a near constant rate for the past fifty years, as shown in Figure 1 adapted from [4]. The data are collected from engine manufacturers based on current designs and forecasts for the next ten years. The pressure ratio is plotted against the year of certification of each engine. The pressure in modern combustors is now exceeding values of 50-60 atm at sea level, and 20-25 atm at high altitude, and even higher values are expected for the future generation of gas turbines. During typical operation in a jet engine, fuel is injected at supercritical conditions during takeoff and landing, and near critical or subcritical conditions during climbing and cruise. Furthermore, aeroderivative gas turbines have recently seen widespread application in the power generation industry, increasing the need for an accurate assessment of NO\textsubscript{x} emissions during supercritical combustion. Supercritical fuel injection and mixing has become a relevant issue for many propulsion and power generation applications.

In jet engines fuel is injected in the form of liquid droplets into the hot and elevated pressure environment of the combustion chamber. The fuel usually enters the combustor at high pressure, but low temperature and is heated as it moves toward the hot combusting region. Droplets can undergo three different evaporation regimes depending on the ambient pressure and temperature in the combustor. The three regimes are represented on the phase diagram in Figure 2, adapted from Banuti et al. [5].

The temperature and pressure are normalized using the critical value: \[ T_r = T/T_c, \] and \[ p_r = p/p_c. \] The figure shows the coexistence line separating the liquid and gas phases at subcritical conditions. The so-called Widom line is an extension of the coexistence line in the supercritical region, separating the gas-like and liquid-like domains. Subcritical evaporation occurs when the conditions in the combustor are below the critical pressure and temperature of the fuel (\( T_r < 1, P_r < 1 \)). At increasingly high ambient pressure and near the critical point real gas effects cannot be neglected and transient effects become dominant. Near-critical evaporation is characterized by increased rate of surface heating and varying saturation temperatures. When fuel is injected at supercritical conditions, new mechanisms become rate-controlling factors for mixing...
and heat transfer. The supercritical state causes intermolecular forces to become dominant, leading to major changes in some relevant fluid properties, so that all aspects of the combustion process depart from the better-known subcritical behavior.

There are several challenges associated with the fundamental characterization and modeling of fluids at supercritical conditions. Fluid properties display highly non-linear behavior in the proximity and above the critical point. This is caused by the more dominant repulsion and attraction forces between molecules. The fluid undergoes dramatic variations in density and specific heat that are very sensitive to pressure and temperature variations. This non-linear behavior makes the choice of an adequate Equation of State (EOS) model critical. The accuracy and thermodynamic consistency of such models is still uncertain and the characterization of the non-linear fluid behavior remains a long-standing problem [6].

![Phase diagram illustrating different evaporating regimes.](image)

**Figure 2:** Phase diagram illustrating different evaporating regimes.

Sirignano [7] and Lafon et al. [8] report that the solubility of ambient gases into the injected supercritical fuels increases at high pressure. Once the fluid reaches supercritical pressure surface tension vanishes, mixing becomes a diffusion driven process and there is no clear interface between the liquid and the gas phase. The “critical interface” is often defined as the region where the fluid temperature is equal to the critical temperature, but there is no universal consensus on this definition.

The modeling of supercritical fuel injection in jet engines requires the solution of several length and time scales. Combustion instabilities act on a system level requiring the modeling of acoustic and combustor scales. Production of harmful pollutants in jet engines occurs at the molecular level. In supercritical fluids and fluids near saturation intermolecular forces cannot be neglected. The large variety of scales involved leads to high computational cost of numerical simulations. Hickey et al. [9] and Mueller et al. [10] developed high-fidelity calculations to simulate supercritical fuel injection. Numerical instabilities are common at the “critical interface” due to large variations of thermophysical properties. Discrepancies of the predicted fuel density as large as 50% are not uncommon in numerical studies, clearly pointing out limitations of current modeling techniques.

Experimental data on supercritical fuel injection are scarce due to the cost and complexity of measurements at high pressure and temperature. Among the many substantial contributions to experimentally characterize the dynamics of supercritical and transcritical processes, the works of Chehrouri [11] and Bellan [12] stand as the most comprehensive and recent reviews of experimental campaigns. Droplet evaporation has been extensively studied for over sixty years. Most of the experimental work, however, has solely dealt with subcritical evaporation or cases in which at most only one state parameter (temperature or pressure) was above the critical point. The major reason for the limited dataset is the challenge with the definition of the “critical interface” due to the vanishing surface tension at supercritical state, which makes standard optical methods inapplicable for distinguishing the supercritical and the subcritical states. In many cases the supercritical state is not reached before the droplet completely evaporates even in a supercritical environment. Matlosz et al. [13] conducted experiments with isolated hexane droplets with diameters around 1 mm evaporating in quiescent nitrogen or argon at reduced temperatures of $T_r = 1.08$ and reduced pressures of up to $P_r = 3.41$. The study provided both droplet diameter and surface temperature time-varying data, but included only limited data points. Tseu et al. [14] covered reduced ambient temperatures up to 1.43 and pressures up to 3.65 but also had limited data resolution. Sato et al. [15], Morin et al. [16] and Ghassemi et al. [17] conducted detailed measurements of evaporating droplets in nitrogen, but focused mainly on subcritical cases. Nomura et al. [18] provides a database of measurement of heptane droplets evaporating in nitrogen at subcritical and near-critical conditions that have been widely used for the validation of numerical models. Chehrouri et al. [19] investigated supercritical jet injection in various configuration useful for rocket propulsion applications. The authors conducted density measurements using Raman scattering and investigated the effects of pressure perturbations on the jet dynamics at different temperature and pressure. Rachedi et al. [20] [21] examined the behavior of a real jet fuel (JP-10), and compared it to Zeaton et al.’s [22] carbon dioxide data. Their results showed that carbon dioxide could be used as a surrogate fluid for JP-10.

General-purpose computational fluid dynamics based on solving the Reynolds-averaged Navier-Stokes (RANS) equations has become standard in the aerospace industry. Spray simulations utilize a Eulerian-Lagrangian formulation in which droplets are treated as discrete, point-like particles. Traditional evaporation modeling capabilities in current design tools are mostly limited to subcritical conditions, thus not properly capturing the changes in evaporation behavior occurring near and past the critical point. There is a need for a more general evaporation framework capable of modeling subcritical, near-critical and supercritical regimes.
2. SCOPE OF PAPER

This paper presents a comprehensive assessment of near-critical and supercritical effects in single droplet evaporation at conditions characteristic of modern liquid-fueled combustors. The work aims to extend existing spray modeling capabilities to account for real-fluid effects at near-critical and supercritical conditions. The main objectives are (i) to determine the scaling laws and the underlying mechanisms for droplet evaporation at high pressure and temperature, (ii) to establish a droplet evaporation model valid at near-critical and supercritical conditions, (iii) to validate the model with experimental data, (iv) to assess whether a single-component fluid can be used as a fuel surrogate for modeling purposes, and (v) to estimate the impact of real gas effects on spray evaporation at conditions characteristics of modern combustors.

It will be shown that for droplets in quiescent environment the transient and quasi-steady evaporation rates vary exponentially with Lewis number. The analysis demonstrates that subcritical evaporation models overestimate transient evaporation and underestimate quasi-steady evaporation, with discrepancies up to 70% at near critical and supercritical conditions. Temperature profiles are typically under-predicted and fuel vapor concentrations are over-predicted in standard spray calculations with subcritical evaporation models, affecting the prediction of combustion instabilities and pollutant formation.

3. TECHNICAL APPROACH

Scaling analysis is applied to the case of an isolated evaporating droplet in a quiescent environment to determine the non-dimensional groups governing the evaporation mechanism at subcritical, near-critical and supercritical conditions. The scaling analysis reveals dependence of the evaporation rate on Lewis number based on droplet surface temperature. A first-principles numerical model is constructed from the non-dimensional form of the governing equations and used to derive an improved evaporation model valid at near-critical and supercritical conditions. A detailed description of the model is included in the appendix. The model consists of discretized mass, momentum, energy and species conservation, and the caloric and equation of state (EOS) model in non-dimensional form for the liquid and gas phases. Matching conditions are used at the interface and the fluid properties are defined using the NIST RefProp software [23]. A first-order accurate, finite-difference implicit scheme is used. First order spatial and time derivatives are approximated with two-point backward difference in the liquid phase and forward difference in the gas phase. Second order flux derivatives are calculated by applying a central-difference discretization twice. The system is solved iteratively with a Newton-Raphson method. Grid independence was determined with a series of refinements.

The model is validated against existing experiments at subcritical and near critical conditions, and then extended to supercritical conditions. A matrix of test cases is constructed as indicated in Table 1 by varying the ambient temperature and pressure while keeping the droplet temperature fixed, consistent with the experiments by Nomura et al. [18]. Temperature profiles are verified through comparison with high-fidelity calculations at subcritical conditions.

High-fidelity calculations using the commercial solver Fluent are used to assess the impact of the newly developed model on spray evaporation in the subcritical, near critical and supercritical regimes. More details of the numerical method can be found in [24]. The computational approach is based on a finite-volume method using a pressure based, implicit, compressible formulation with a second order spatial discretization. RANS calculations are performed and the governing equations are closed through the two-equation k-ω shear stress transport (SST) turbulence model by Menter [25]. Multiphase calculations are conducted using the built-in Eulerian-Lagrangian model that treats droplets as point-like particles [24]. The NIST Reference Fluid Thermodynamic and Transport Properties Database (RefProp) equation of state model, defined by [23], is incorporated in the CFD solver in the form of lookup tables [26]. This approach has been validated in other works through comparison with other EOS models [29].

| Case | P_{amb} [bar] | T_{amb} [K] | P_r | T_r | Le |
|------|---------------|--------------|-----|-----|----|
| 1    | 1             | 471          | 0.04| 0.87| 8.61|
| 2    | 1             | 648          | 0.04| 1.20| 9.56|
| 3    | 5             | 556          | 0.18| 1.03| 1.78|
| 4    | 5             | 655          | 0.18| 1.21| 1.90|
| 5    | 10            | 669          | 0.37| 1.24| 0.95|
| 6    | 20            | 656          | 0.73| 1.24| 0.45|
| 7    | 30            | 567          | 1.10| 1.05| 0.16|
| 8    | 30            | 650          | 1.10| 1.20| 0.27|

Table 1 Summary of ambient and initial conditions used for the model assessment.

4. SCALING ANALYSIS AND NON-DIMENSIONAL GROUPS

A scaling analysis of the equations governing single droplet evaporation determines the relevant non-dimensional groups that characterize the process. The different physical mechanisms involved are defined for both steady and transient evaporation by the time scales at which the different processes become dominant.

The analysis assumes that droplets are perfectly spherical, reducing the evaporation process to one spatial dimension. This assumption is valid for droplets evaporating in typical aero-engine applications. During injection in the combustor, droplet fragments of different shapes and dimension form, following...
the primary and secondary atomization process. Aerodynamic forces can lead to stretching and thinning of the droplets, however, as the fragments became smaller, surface tension stabilizes the droplets into spherical shapes. It is assumed that the droplets consist of a single-component fluid, neglecting the solubility of the ambient gas in the liquid fuel. Temperature gradients and concentration gradients (Soret and Dufour effects) due to fluid composition are also neglected. These might be relevant for some evaporation processes in rocket engine applications, as pointed out by Yang et al. [27], but are beyond the scope of the present work. It is assumed that mass diffusion fluxes follow Fick’s law and energy diffusion fluxes follow Fourier’s law. Viscous dissipation, buoyancy, compressible, radiation and kinetic effects are not considered. The droplet is assumed in a quiescent environment, representative of the case of small droplets transported by the flow.

![](image)

**Table 2** Characteristic time scales and associated physical processes.

| Process                  | Characteristic Time |
|--------------------------|---------------------|
| Advection                | $t_{adv} = R/u$     |
| Thermal Diffusion        | $t_{th} = R^2/\alpha$ |
| Mass Diffusion           | $t_m = R^2/D$       |

Two additional timescales characterize the droplet transient heating process: the heating time, and the evaporation time. In a jet engine fuel is usually injected at subcritical temperature into the hot, elevated pressure environment of the combustor. As the droplet is immersed into the hot gas, its surface temperature rapidly rises at first and then gradually increases at a lower rate until either reaching the saturation temperature set by the ambient gas pressure or constantly increasing to critical temperature. This is schematically shown in Figure 3.

![Figure 3](image)

**Figure 3** Time history of surface temperature during droplet heating in different regimes.

The system of mass, momentum, energy, species mass fraction conservation, and the caloric equation of state for the liquid and gas phase are expressed in non-dimensional form. A more detailed description of the scaling analysis is given in the appendix. The scaling analysis reveals three characteristic time scales associated with the evaporation process defined in Table 2: the advection time scale, the thermal diffusion time scale and the mass diffusion time scale. The thermal and mass diffusivity refer to the phase of interest, meaning that to determine the thermal diffusion time scale of the droplet the liquid thermal diffusivity is used, $t_{th} = R^2/\alpha_l$. The ratios of these timescales define three dimensionless groups that characterize the relative importance of the advection, thermal diffusion and mass diffusion processes: the Péclet mass transfer number, the Péclet thermal transfer number and the Lewis number as indicated in Table 3.

| Non-dimensional Number     | Interpretation                        | Expression              |
|-----------------------------|---------------------------------------|-------------------------|
| Péclet Mass Transfer Number | Adveotive/Mass Diffusion              | $Pe_m = \frac{t_m}{t_{adv}} = \frac{uR}{D}$ |
| Péclet Thermal Transfer Number | Adveotive/Thermal Diffusion          | $Pe_{th} = \frac{t_{th}}{t_{adv}} = uR/\alpha$ |
| Lewis Number                | Thermal/Mass Diffusion                | $Le = \frac{t_m}{t_{th}} = \frac{\alpha}{D}$ |
| Reduced frequency heating   | Heating/Evaporation Timescales        | $\omega_e = \frac{t_{th}}{t_e}$ |
| Fourier Number              | Non-dimensional Evaporation Time      | $Fo = \frac{\alpha t_e}{R^2}$ |

**Table 3** Non-dimensional parameters governing single droplet evaporation.
corresponding to the saturation value. At increasingly high pressure and near the critical point, real gas effects cannot be neglected. The droplet surface temperature continuously rises during the entire droplet lifetime and never reaches the critical value. The rate of surface heating increases with ambient temperature and pressure. In the supercritical evaporation regime, the droplet surface temperature rises until reaching the critical value. The droplet heating time $t_h$ is defined as the time required to reach the saturation or critical temperature, as indicated in Figure 3. At near critical conditions the heating time is defined as the time required to reach the saturation temperature for the given fuel vapor concentration at the droplet surface. At supercritical conditions there is no real interface between the fuel and the ambient gas, however, the critical interface defined as the locus of points with temperature equal to the critical temperature of the fuel is useful to determine the timescales associated with the problem. The Biot number of evaporating droplets, $Bi = \frac{h_{conv} d}{\lambda_l}$, varies from 0.5 at reduced temperature of 0.6, up to 1.5-2.0 for reduced temperature of 1 [28], meaning that temperature gradients inside the droplets are not negligible near critical conditions. The initial surface temperature rise and transient droplet heating are driven by thermal diffusion in the gas and liquid phases, respectively. The energy the droplet receives from the surroundings via convective heat transfer internally heats the droplet and leads to evaporation. The initial driving force for the surface temperature increase is heat diffusion in the gas phase as internal droplet heating requires more energy. The droplet evaporation time $t_e$ is defined as the time required for the entire droplet to evaporate. The ratio of the heating and evaporation times yields the reduced frequency $\omega_t$, which represents the relative importance of transient droplet heating effects during the evaporation process. The scaling analysis also identifies the dimensionless evaporation time or Fourier number, as indicated in Table 3.

By utilizing fluid properties from RefProp at saturation conditions for a range of reduced ambient pressures, the analysis indicates that the droplet heating time becomes a larger portion of the total evaporation time at near-critical and supercritical conditions, yielding larger $\omega_t$. This is consistent with other models in literature as reported by Sirignano [7]. Liquid heating time, $t_h$, is of the order of evaporation time, $t_e$, and $\omega_t$ increases with ambient conditions approaching the critical point, so droplet evaporation becomes increasingly a transient and thermal diffusion dominated process. Thus $t_h$ is an appropriate scale to characterize the droplet lifetime at near-critical and supercritical conditions.

The scaling analysis indicates that the Lewis number rapidly decrease at near critical conditions. The diffusion time scales as $R^2/\alpha$ and, consequently, droplet heating can be estimated as the time for a thermal diffusion wave to propagate from the liquid/gas interface to the droplet center, or $t_h = R^2 / \alpha_{liq}$, where $\alpha_{liq}$ is the thermal diffusivity of the liquid phase. Similarly, gas heating time is of the order of $R^2 / \alpha_{gas}$ with $\alpha_{gas}$, the thermal diffusivity of the gas phase. The initial surface temperature rise occurs on a time scale of $R^2/\alpha_{gas}$. As the fluid reaches critical conditions, thermal diffusion becomes dominant, leading to reduced Lewis numbers.

Data from two sets of experimental measurements are taken to assess the dependence of evaporation parameters on $\omega_t$ and Lewis number. The data correspond to subcritical and near-critical evaporation measurements from Nomura et al. [18] and supercritical results from Matlosz et al. [21]. The two studies use different fuels (heptane and hexane) over different ranges of ambient pressure and temperature values. The results corroborate the hypothesized dependencies of evaporation regimes on $\omega_t$ and Lewis number. Figure 4 shows increasing relevance of transient heating at large Lewis numbers. The computed Lewis number is plotted versus non-dimensional evaporation time, $F_o$, in Figures 5. The results indicate two characteristic regimes in agreement with the predictions of the scaling analysis. At low temperatures and pressures within the subcritical range, evaporation time rises with Lewis number and transport of fuel vapor in the gas phase is increasingly governed by thermal diffusion. In contrast, at supercritical temperatures and pressures, fuel vapor behavior in the surroundings gas mixture is dominated by mass diffusion. Conversely, surroundings gas behavior is thermal-diffusion-dominated. Transient liquid heating also becomes a larger part of the evaporation process. In addition, in the supercritical region evaporation seems to approach asymptotic behavior, indicating a balance between the different rate-controlling factors.

Based on the results of the analysis, it is hypothesized that the Lewis number and $\omega_t$ are the key parameters to characterize evaporation in the subcritical, near-critical and supercritical regimes.
5. FIRST-PRINCIPLES BASED DROPLET EVAPORATION MODEL

The first-principles model aims to characterize transcritical droplet evaporation and defines correction factors that can be applied to traditional subcritical vaporization approaches to model the evaporation behavior at subcritical, near-critical and supercritical conditions. The model is tested using the ideal gas EOS and real gas properties from the NIST RefProp software to assess the impact of real gas effects on the predicted evaporation rate and quantify discrepancies caused by using ideal gas models. A series of validations of the first-principles solver are conducted, comparing the results with numerical and experimental data of a single droplet in various environments. The temperature distribution during the droplet transient heating process at subcritical conditions corresponding to Case 1 of Table 1 is compared with the results using the commercial code ANSYS Fluent. The radial temperature distribution at a non-dimensional time \( t^* = 0.0075 \) in Figure 6 indicates agreement of the first-principles based numerical model and Fluent within 1.15%.

The evaporation rate is compared with experimental measurements from Nomura et al. [18] in Figures 7 and 8. The droplet conditions are representative of subcritical and near-critical conditions corresponding to Case 1-6 in Table 1. The model validation is conducted with subcritical and near-critical test cases due to the lack of experimental data at supercritical conditions caused by challenges in defining the “critical interface”. The quasi-steady regime after the droplet reaches saturation at ambient pressure is explored first. During this period the droplet surface area decreases linearly with time at a constant evaporation rate. The data are presented in the form of the non-dimensional evaporation rate

\[
K_{ev}^* = K_{ev}/a_{amb}.
\]

The evaporation rate \( K_{ev} \) is defined as the slope of the curve \( d^2/dz^2 \) versus \( t/d_0^2 \), as indicated by Sirignano [7]. The dashed lines represent exponential fits for each dataset. The non-dimensional evaporation rate increases with decreasing Lewis number, with the rate of increase accelerating when approaching the critical point.

The main driving force is the increase in ambient pressure. In particular, at subcritical pressures below \( P_r = 0.1 \), the non-dimensional evaporation rate does not vary much with ambient temperature, being on the order of \( 10^{-3} \), as illustrated by the two cases at high Lewis number. As ambient pressure rises, the impact on evaporation increases and the non-dimensional evaporation rate grows to values on the order of \( 10^{-2} \). Finally,
when the ambient pressure approaches the critical point at $P_r = 0.73$, the rate increases further to values on the order of $10^{-1}$.

Figure 8: Percentage difference between real fluids, ideal fluids models and experiment [18] showing increasing real-fluid effects at decreasing Lewis number.

The real-fluid, first-principles approach shows good agreement with the experimental data. The percentage difference between the models and the experiments is shown in Figure 8. The real-fluid model yields 20% reduced evaporation rate than the experimental values at the lowest Lewis number. This is consistent with the observations of Yang et al. [28], which suggest that fiber conduction and radiative absorption in the droplet experiments increase the evaporation rate. In addition, the discrepancy between the real-fluid solution and experiment increases with ambient pressure and decreasing Lewis number. This is likely due to increasing inaccuracy in determining fluid properties at high pressures near the critical point and to difficulties in performing optical measurements to locate the liquid/gas interface as the fuel surface tension decreases. As expected, the ideal-fluid model yields similar results to the real-fluid and experimental data only at low subcritical pressures, corresponding to high Lewis numbers. Discrepancies up to 66% are found in near-critical conditions at $P_r = 0.73$. Exponential fits are indicated by dashed lines in Figure 7. The results indicate that the quasi-steady evaporation rates vary exponentially with the Lewis number.

6. ASSESSMENT OF SINGLE DROPLET EVAPORATION

The first-principle model for transcritical and supercritical evaporation is assessed in the case of a single non-convective heptane droplet suspended in nitrogen. The model is implemented in ANSYS Fluent and compared with the built in evaporation model and experimental data from Nomura et al. [18]. The numerical setup consists of a rectangular domain with the heptane droplet placed in the center. The boundaries of the domain are located over 300 droplet diameters away to avoid any interference. The surroundings are representative of a quiescent droplet evaporation test, with no relative velocity between the droplet and the ambient gas. The results are presented in the form of evolution of the droplet diameter in time in Figures 9-12. Cases 3, 5, 6 and 7 of Table 1 are presented here. The ambient temperature and pressure are representative of subcritical, near critical and supercritical evaporation.

Figure 9: Droplet diameter time history for case 3 at subcritical conditions, $P_r=0.18$ and $T_r=1.03$.

Figure 10: Droplet diameter time history for case 5 at subcritical conditions, $P_r=0.18$ and $T_r=1.24$.

Figure 9 and 10 show the results of the cases with subcritical temperature and pressure. The results from the first-principles model are within 5% of the experiments, while the built-in evaporation model in Fluent yields discrepancies up to 23%, largely overestimating the evaporation rate of the droplets at subcritical conditions. Figure 11 shows the results for near critical conditions corresponding to Case 6. The first-principle model yields a 5% larger $d_d^2/d_t^2$ compared to the experiments, while the subcritical evaporation model built-in in Fluent

The results from the first-principles model are within 5% of the experiments, while the built-in evaporation model in Fluent yields discrepancies up to 23%, largely overestimating the evaporation rate of the droplets at subcritical conditions. Figure 11 shows the results for near critical conditions corresponding to Case 6. The first-principle model yields a 5% larger $d_d^2/d_t^2$ compared to the experiments, while the subcritical evaporation model built-in in Fluent
overestimates evaporation by 27% and under-predicts droplet lifetime. This is consistent with what was found for the ideal-fluid models during transient evaporation. Finally, Figure 12 shows the comparison at supercritical conditions. In this case the results are not compared to experiments due to the lack of measurements at supercritical conditions caused by challenges in determining the “critical interface”, as indicated by Nomura et al [18]. Nevertheless, the results are consistent with what was observed at near critical conditions and indicate that standard evaporation models overestimate the rate of phase transition compared to the first-principles model.

Figure 11: Droplet diameter time history for case 3 at near critical conditions, Pr=0.73 and Tr=1.21.

Figure 12: Droplet diameter time history for case 3 at supercritical conditions, Pr=1.1 and Tr=1.05.

7. SPRAY CALCULATIONS

The non-dimensional evaporation rate dependencies developed using the first-principles model are implemented in a spray calculation framework in ANSYS Fluent [24]. The influence of different fluid properties models is investigated using three EOS models: ideal-fluid, Peng-Robinson (PR), and NIST RefProp model. The difference between traditional evaporation models and the first-principles model are also assessed.

Figure 13: Schematic of crossflow setup with boundary conditions used

The assessment of the spray calculations is conducted by looking at the case of a spray in crossflow. Figure 13 shows a schematic representation of the test case. Heptane droplets are injected in nitrogen gas flowing at 2 m/s. The conditions of the test case are consistent to other spray into cross flow experiments and calculations found in literature [7][17]. The velocity is selected so that the droplet residence time in the domain is one order of magnitude larger than the evaporation time. The domain consists of a duct with rectangular section, with the heptane droplets injected in the direction normal to the main nitrogen flow. The diameter if the injector D=0.1mm is representative of typical spray injector orifices. Droplets enter the domain through an injector of diameter D and length L/D=4. The duct height and length are 750 and 4060 times the injector diameter respectively. The width of the flow channel is z/D = 1250. The calculations are conducted using mass flow inlet and a pressure boundary at the outlet.

The conditions of the ambient gas are chosen so that all three evaporation regimes are investigated, by changing the temperature and pressure of the nitrogen gas while maintaining fixed the droplet temperature consistent with the conditions of isolated droplet experiment treated in section 5 and 6 of this paper. Five cases are considered, corresponding to Case 1, 4, 5, 6 and 7 in table 1. Three cases are subcritical, one near critical and one is supercritical.

The liquid injection is modeled with the plain orifice atomizer model in Fluent which determines droplet diameter and velocity distributions based on the L/D ratio, surface tension, and mass flow rate. A structured mesh with 1.3 million elements is used. The mesh is refined in the area downstream of the liquid jet inlet and consists of cells with minimum dimensions Δx/D =3, Δy/D =9, and Δz/D =3.
Equation of State Model Assessment:

The total vapor mass fraction is compared among the different models across several cross sections downstream of the injector. The total vapor fraction at several cross planes are plotted versus the axial coordinates in Figures 14-18. The data show that the PR model matches the RefProp results only at subcritical conditions, with the discrepancies between the two EOS models increasing at supercritical conditions. The ideal-fluid model, in contrast, overpredicts evaporation with an increasing error as the ambient pressure increases. The vapor mass fraction is plotted versus the transverse direction at two cross sections: one in the near field at x/D=200 and one in the far field at x/D=1800 downstream of the injector in Figure 19, 20 and 21. The overprediction of the ideal model is more pronounced near the injector where fuel vapor concentrations are higher, yielding up to 7% discrepancies between the ideal model and Refprop.

![Figure 14: Heptane vapor fraction along midline in Case 1. Fuel injected into ambient condition T_r=0.87 and P_r=0.04.](image1)

![Figure 15: Heptane vapor fraction along midline in Case 4. Fuel injected into ambient condition T_r=1.21 and P_r=0.18.](image2)

These results are in agreement with the first-principles analysis in Section 5, which indicated that ideal-fluid modeling overestimates transient evaporation. In fact, the convective heat transfer in a crossflow injection increases the heat received by droplets and hence the evaporation rate. Thus the transient heating period becomes a larger part of the droplet lifetime and droplets might evaporate completely before reaching saturation at ambient pressure. The largest discrepancies between the different models are encountered at supercritical conditions, shown in Figure 18. In this case heptane is injected at supercritical pressure, and subcritical temperature in an environment at supercritical temperature. In Figure 18 and the near field up to x/D=800 the concentration of supercritical heptane is highest for the ideal model and lowest for the PR model, with discrepancies of 8% between the PR and Refprop models, and 17% between the ideal and Refprop models. The trend is inverted in the far field at x/D=1800, where Refprop indicates the highest heptane concentration, and the PR model and ideal model show 6% and 25% lower concentrations compared to Refprop, as shown in Figure 21. Trends are inverted for the subcritical case shown in Figure 20.

![Figure 16: Heptane vapor fraction along midline in Case 5. Fuel injected into ambient condition T_r=1.24 and P_r=0.37.](image3)

![Figure 17: Heptane vapor fraction along midline in Case 6. Fuel injected into ambient condition T_r=1.24 and P_r=0.73.](image4)

The difference between ideal and real-fluid models increases with pressure and temperature. The comparison between the different fluid property models suggests that the PR model can potentially be used as an alternative to the RefProp database at subcritical conditions. At near critical and supercritical conditions, the analysis indicates that RefProp provides the highest fuel concentration among the models.
Figure 18: Supercritical heptane fraction along midline in Case 7. Fuel injected into ambient condition $T_r=1.05$ and $P_r=1.1$.

Figure 19: Heptane vapor fraction in a cross section at $x/D=200$ in Case 1. Fuel injected into ambient condition $T_r=0.87$ and $P_r=0.04$.

First Principles Model Assessment:

The first-principles model was assessed with spray calculations. In each case, three combinations of fluid-property model and evaporation model are evaluated: Fluent evaporation model with ideal fluids, Fluent evaporation model with RefProp fluid properties, and first-principles model evaporation with RefProp real-fluid data, called here “transcritical model”. The results for the averaged fuel vapor mass fraction at different locations downstream of the injector indicate that the subcritical evaporation model in Fluent typically predicts higher evaporation than the transcritical model as ambient pressure increases. Consequently, traditional modeling results in higher fuel vapor concentrations and lower gas phase temperatures. The downstream development of the fuel vapor mass fraction and temperature transverse profiles are shown in Figure 22 and Figure 23, respectively, at $x/D=1800$ downstream of the injector. The results suggest that subcritical models predict higher convective heat transfer and lower gas temperatures than the transcritical model. Evaporation rate behavior, in contrast, varies with distance. Near the injector, at high temperatures and mass fractions, the transcritical model indicates lower evaporation and lower fuel vapor concentrations. Differences of up to 2% in the temperature distribution due to the increased fuel concentration are found between models. As the chemical reaction rate in combustion has an exponential dependence on the temperature, even small changes in temperature can have tremendous impact on the combustion process. In particular, this might affect NOx production in jet engines, leading to erroneous estimations of emissions in numerical calculations.

Figure 20: Supercritical heptane fraction in a cross section at $x/D=1800$ in Case 1. Fuel injected into ambient condition $T_r=0.87$ and $P_r=0.04$.

Figure 21: Supercritical heptane fraction in a cross section at $x/D=1800$ in Case 7. Fuel injected into ambient condition $T_r=1.05$ and $P_r=1.1$.

8. CONCLUSIONS

This paper presents a comprehensive assessment of near-critical and supercritical effects in single droplet evaporation at conditions characteristic of modern liquid-fired combustors. The work develops spray modeling capabilities to account for real-fluid effects at near-critical and supercritical conditions. The major outcomes can be summarized as follows:

1) A scaling analysis for single droplet evaporation at subcritical and supercritical conditions in a non-convective environment suggests that the key parameter to characterize the evaporation process is the Lewis number and the ratio of droplet heating time and evaporation time. This result indicates that a single-component fluid can be potentially used as a surrogate for jet fuel for modeling purposes.

2) A first-principles modeling framework of near-critical and supercritical droplet evaporation is established and
validated against published experimental data. The results suggest that both transient heating and quasi-steady evaporation rates vary exponentially with Lewis number.

3) First-principles modeling indicates that subcritical ideal-fluid models increasingly overestimate transient evaporation and underestimate quasi-steady evaporation with increasing ambient pressure. The discrepancy with the measured evaporation rate is up to 70% at near-critical conditions.

4) Comparison between first-principles model and the built-in Fluent spray models suggests that classical subcritical models lack real-fluid property and non-uniform temperature profile characterization at near-critical conditions, leading to over-predicted evaporation.

ACKNOWLEDGMENTS

This research was funded by Mitsubishi Heavy Industries Takasago R&D Center, which is gratefully acknowledged. In particular, the authors would like to thank Dr. Eisaku Ito, Dr. Yuasa and Mr. Awasthi for their support.

Figure 22: Fuel vapor mass fraction cross-sectional distributions at x/D = 1800 downstream of the injector.
Figure 23: Gas temperature cross-sectional distributions at x/D = 1800 downstream of the injector.

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9. APPENDIX

Scaling Analysis:
The physical length scale associated with droplet evaporation is the time-varying droplet diameter, R. Thus if radial distance scales with R, and density and time scale with some characteristic values ρ and t, the different terms in the continuity equation scale as follows:

\[
\frac{\partial (\rho r^2)}{\partial t} + \left( \frac{\partial \rho r^2 u}{\partial r} \right) = 0.
\]

\[
\frac{\rho R^2}{t} = \rho u R
\]

For both terms being equally important, the characteristic time scale is \( t \sim R/u \) i.e. advection velocity scales as \( u \sim R/t \).

Similarly, the different terms in the species balance equation scale as:
\[
\frac{\partial (\rho Y_F r^2)}{\partial t} + \frac{\partial (\rho Y_F r^2 u)}{\partial r} - \frac{\partial}{\partial r} \left( \rho Dr^2 \frac{\partial Y_F}{\partial r} \right) = 0,
\]

which defines the characteristic time \(R^2/D\). Various terms in the energy equation scale as:

\[
\frac{\partial (\rho r^2)}{\partial t} + \frac{\partial (\rho r^2 u)}{\partial r} - \frac{\partial}{\partial r} \left( \lambda r^2 \frac{\partial T}{\partial r} \right) - \frac{\partial}{\partial r} \left( \rho Dr^2 (h_F - h_{AC}) \frac{\partial Y_F}{\partial r} \right) = 0,
\]

where \(R^2/\alpha\) is the resulting time scale, \(\alpha = \lambda / \rho c_p\) being the thermal diffusivity of the phase under consideration. Further details are included in [26].

First Principles Numerical Model:

The framework is developed in MATLAB. A schematic of the numerical domain is shown in Figure 25. A spherical coordinate system is utilized. The liquid phase is defined as extending from the droplet center to the droplet surface. The gas domain is the region outside the interface extending to an arbitrarily set far-field boundary. The gas-liquid interface itself provides matching conditions between the liquid and gas phases. The equations are written in non-dimensional form as follows:

\[
r^* = \frac{r}{R_0}, \quad R^* = \frac{R}{R_0}, \quad t^* = \frac{\alpha_0 t}{R_0^3}, \quad u^* = \frac{u R_0}{D_{0,\alpha}}, \quad T^* = \frac{T - T_{\infty}}{T_{\infty} - T_0},
\]

\[
\rho^* = \frac{\rho}{\rho_{0,j}}, \quad h^* = \frac{h}{h_{0,j}}, \quad c_p^* = \frac{c_p}{c_{p_{0,j}}}, \quad \lambda^* = \frac{\lambda}{\lambda_{0,j}}, \quad D^* = \frac{D}{D_{0,j}}, \quad m^* = \frac{m_{R_0}}{\rho_{0,j} c_{p_{0,j}}},
\]

\[
\frac{\partial (\rho^* r^2 u^*)}{\partial t^*} + \frac{1}{L_0} \frac{\partial (\rho^* r^2 u^*)}{\partial r^*} = 0,
\]

\[
Y_F = 1, \quad Y_{\rho} = \frac{\rho_{0,j}}{\rho}, \quad Y_{c_p} = \frac{c_{p_{0,j}}}{c_p}, \quad Y_{\lambda} = \frac{\lambda}{\lambda_{0,j}}, \quad Y_{D} = \frac{D}{D_{0,j}}, \quad Y_{m} = \frac{m_{R_0}}{\rho_{0,j} c_{p_{0,j}}},
\]

\[
\frac{\partial (\rho^* h^2 r^2 u^*)}{\partial t^*} + \frac{1}{L_0} \frac{\partial (\rho^* h^2 r^2 u^*)}{\partial r^*} + N\frac{\partial}{\partial r^*} \left( \lambda^* r^2 \frac{\partial T}{\partial r^*} \right) - \frac{1}{L_0} \frac{\partial}{\partial r^*} \left( \rho^* D^2 r^2 (h_F - h_{AC}) \frac{\partial Y_F}{\partial r^*} \right) = 0,
\]

and

\[
\frac{\partial (\rho^* r^2)}{\partial t^*} + \frac{10}{L_0} \frac{\partial (\rho^* r^2 u^*)}{\partial r^*} = 0,
\]

\[
\frac{\partial (\rho^* Y_F r^2 u^*)}{\partial t^*} + \frac{10}{L_0} \frac{\partial (\rho^* Y_F r^2 u^*)}{\partial r^*} - \frac{1}{L_0} \frac{\partial}{\partial r^*} \left( \rho^* D^2 r^2 \frac{\partial Y_F}{\partial r^*} \right) = 0,
\]

in the gas domain. The interface matching conditions are:

\[
\rho^* (\frac{1}{L_0} u^* - \tilde{r}^*) = \rho^*_g (\frac{1}{L_0} u^* - \tilde{r}^*) = m^*,
\]

\[
\rho^*_g D^*_g \left( \frac{\partial Y_F}{\partial r^*} \right)_{sg} - \rho^* D^*_l \left( \frac{\partial Y_F}{\partial r^*} \right)_{sl} = L_0 m^*(Y_F, sg - Y_F, sl),
\]

\[
\lambda^* \left( \frac{\partial T^*}{\partial r^*} \right)_{sl} - \lambda^*_g \left( \frac{\partial T^*}{\partial r^*} \right)_{sg} = \frac{1}{J_{a_0} h_{evap} m^*},
\]

with:

\[
L_0 = \frac{\alpha_0}{c_p(T_{\infty} - T_0)},
\]

\[
N_{h_{0,i}} = \frac{c_p(T_{\infty} - T_0)}{h_{0,i}},
\]

\[
J_{a_0} = \frac{c_p(T_{\infty} - T_0)}{h_{evap F_0}}.
\]
these equations (species and energy balances) are second-order partial differential equations, so they require two boundary conditions. The rest of the equations are first-order in $r$ and need only one boundary condition. Thus a total of seven boundary conditions are needed in each domain or fourteen for the whole system. Ten of them are provided by the boundary conditions at the droplet center and the far field and the remaining four from the matching conditions at the interface and surface equilibrium. The remaining equation at the interface is used to determine $R$. 

