Summary

Name: LEANG So Khuong

Title of dissertation for the degree

INVESTIGATION OF DROPLET EVAPORATION CHARACTERISTICS OF CONVENTIONAL AND CARBON-NEUTRAL TRANSPORTATION FUELS UNDER VARIOUS TEMPERATURE AND PRESSURE CONDITIONS

Rising global awareness of climate change and CO_2 emissions drives the shift to alternative energy sources to meet the net-zero target by 2050. Figure 1 shows the global energy-related CO_2 emissions by sector. It highlights industry, coal and gas power plants, and transportation as major contributors, collectively responsible for over 80% of global CO_2 emissions. Transportation accounts for more than half of the oil used and nearly 25% of energy-related CO_2 emissions, which is expected to increase by more than 50% by 2030 and more than double by 2050. The UN Climate Change Conference (COP26) in 2021 emphasized the need for a shift in energy sources to achieve a net-zero pledge, limiting global temperature rise to 1.5℃ by 2050. This shift entails replacing conventional fuels with carbon-neutral alternatives like hydrogen, ammonia, and oxygenated fuels such as biodiesel and hydrotreated vegetable oil (HVO) for compression ignition (CI) engines, alongside an emphasis on enhancing fuel efficiency.

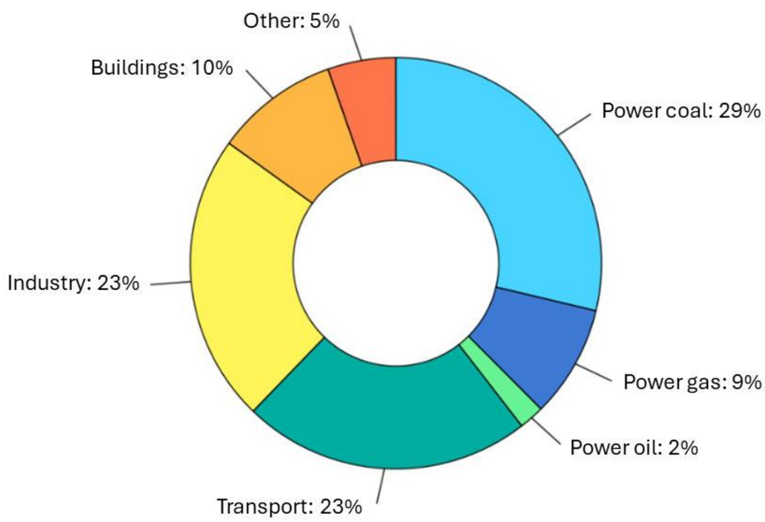


Figure 1 Global energy-related CO_2 emissions by sector.

Hydrotreated vegetable oil (HVO) and ammonia stand out as promising solutions for sustainable transport fuel, offering carbon-neutral attributes that align with environmental goals. Nevertheless, the intricate challenges associated with their physical and combustion properties significantly impact their performance in CI engines, influencing fuel injection efficacy, combustion efficiency, and exhaust emissions (NH_3, NO_x, N_2O, and soot). Addressing these challenges necessitates a comprehensive exploration of spray dynamics, combustion processes, and emission formation for each fuel. Specifically, in spray combustion, physical and chemical phenomena can be observed separately. As shown in Figure 2, the injected fuel penetrates, breaks up, and atomizes. Many fine droplets disintegrate and then evaporate before combustion. If fuel droplets do not evaporate in time, several major issues such as incomplete combustion, knocking and excessive emissions may occur. In previous studies, the evaporation characteristics of various fuels such as biodiesel and diesel, and biodiesel-ethanol blends have been experimentally investigated. However, no experimental studies on single HVO and ammonia droplet evaporation have been reported as of the time this study was conducted. Therefore, single droplet evaporation characteristics of HVO and ammonia fuel were investigated in this study.

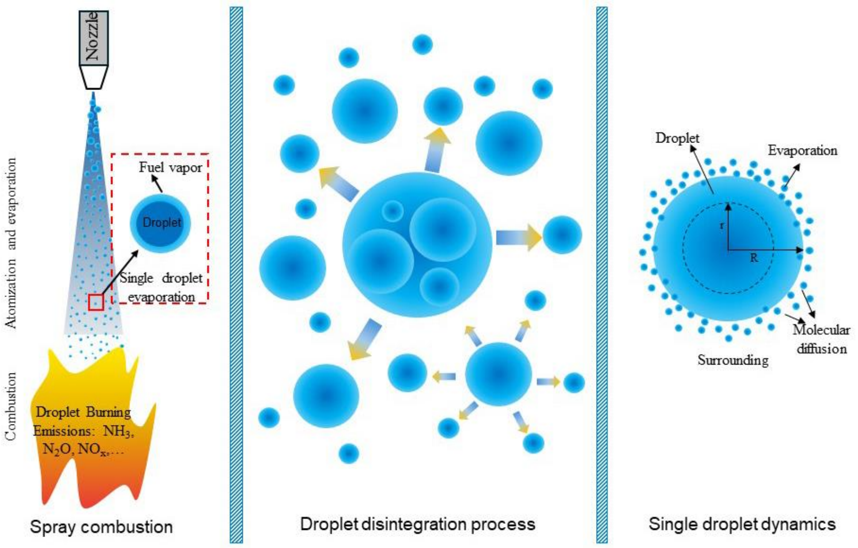
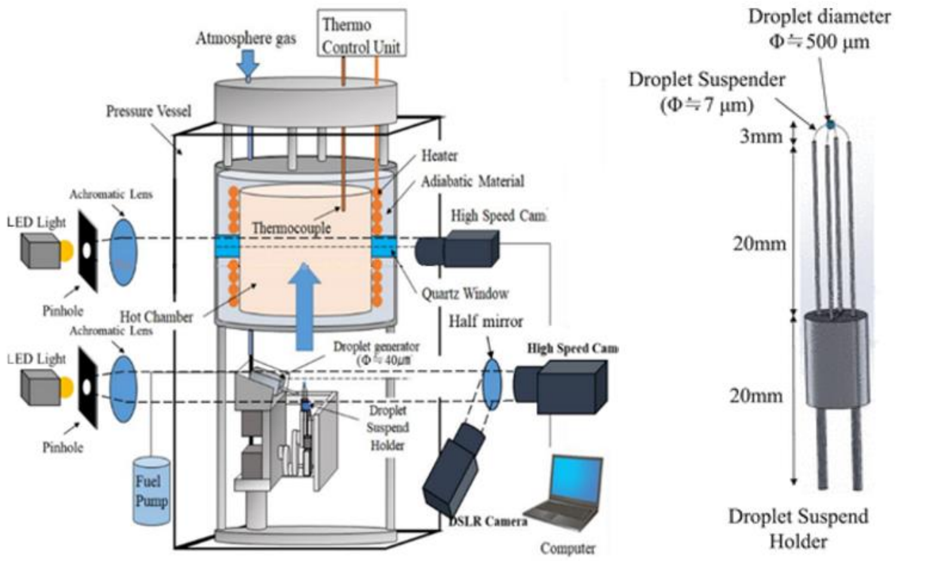


Figure 2 Spray combustion and droplet dynamics

Several experiments were conducted to achieve the objectives of this study. First, surrogate HVO fuels were formulated and surrogate HVO droplet evaporation experiments were performed under high temperatures (573 K-873 K) and pressures (0.1-2.0 MPa) using a conventional experimental setup, shown in Figure 3. The pressure vessel was made of extra super Duralumin (JIS A7075). The top cover of the vessel was equipped with a temperature-controlled hot chamber and droplet generation and insertion mechanisms, as shown in Figure 3a. Before conducting experiments, the vessel was vacuumed and filled with N_2 to observe pure evaporation without a combustion reaction. Then, a microflow pump was used to deliver fuel to the tip of the glass needle (outer diameter: 40 µm). Inside the pressure vessel, the fuel droplet with a diameter in the range of 500±15% µm was then suspended onto the intersection point of two Al_2O_3/SiO_2 fibers with a 7 µm diameter as indicated in Figure 3b. Finally, after droplet generation, the glass needle was evacuated in preparation for the droplet insertion into the hot chamber via an open entrance for the droplet suspender holder. Two high-speed cameras (DITECT, HAS-X) were used to observe the droplet diameter change during both the droplet generation process and the evaporation process.



(a) Droplet evaporation experimental setup (b) Schematic of droplet suspender

Figure 3 Schematic of HVO droplet evaporation experimental apparatus.

Next, a new experimental setup was designed and developed specifically for single ammonia droplet evaporation experiments. Then, ammonia evaporation characteristics were observed both experimentally and numerically at ambient temperatures (298 K to 673 K) and a fixed pressure of 0.95 MPa. The schematic of the experimental apparatus for the ammonia droplet evaporation test is shown in Figure 4. The pressure vessel was made of stainless steel (SUS304). The top cover of the vessel was equipped with a temperature-controlled hot chamber, and droplet generation and droplet elevation mechanisms were connected to the window plate of the pressure vessel. The ammonia cylinder was placed upside down to obtain liquid ammonia. To maintain ammonia in the liquid state, the fuel ammonia pipe was placed into a larger hollow pipe filled with circulating coolant ($T_{coolant}$ = 24 ~ -27°C). It is challenging to conduct droplet evaporation experiments at varying ambient pressures because when the ammonia pipe pressure (P_{pipe}) is larger than the ambient pressure (P_{amb}), liquid ammonia exits the tip of the glass needle like an injected spray. However, when the $P_{pipe} < P_{amb}$, the flow of liquid ammonia is blocked, preventing droplet generation. To perform the droplet evaporation experiment, a single ammonia droplet is continuously generated and then delivered to the hot chamber

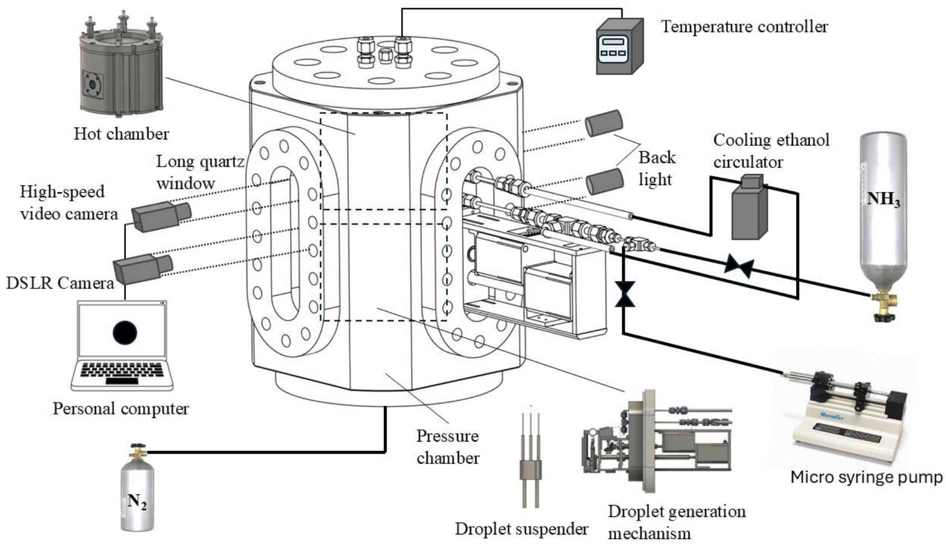
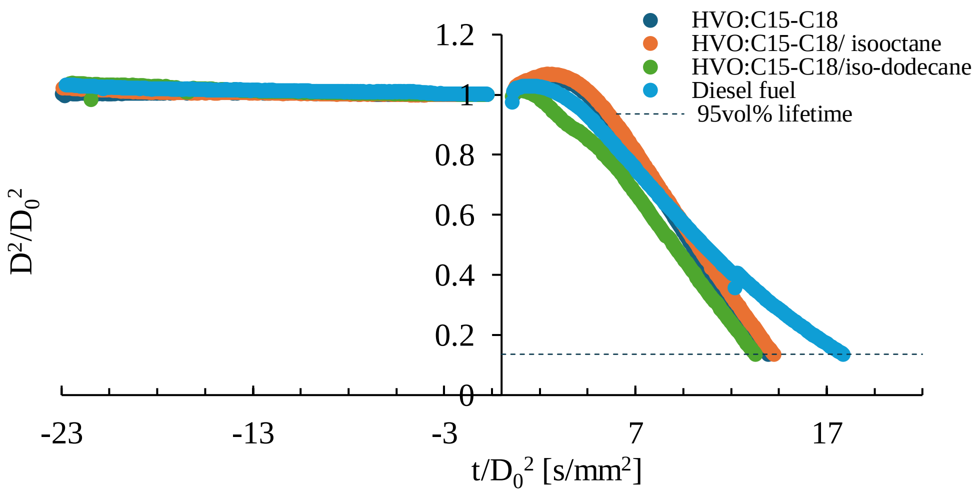
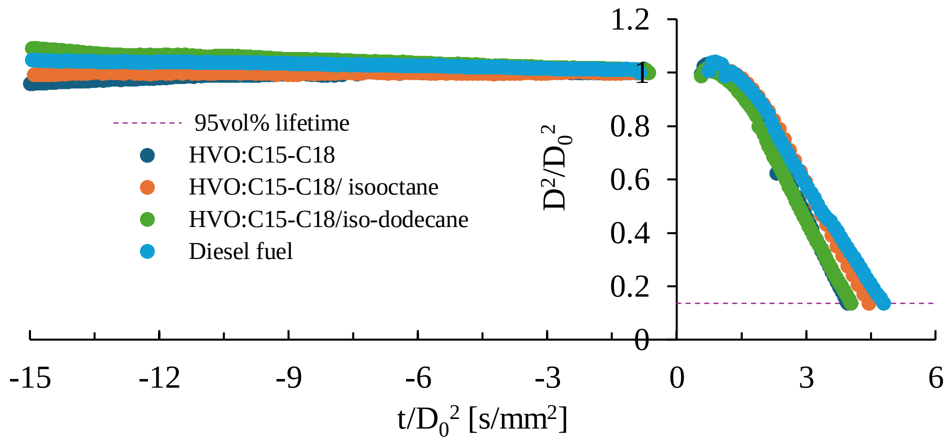


Figure 4 Schematic of droplet evaporation experimental apparatus.

Key parameters such as properties, droplet lifetime, and instantaneous evaporation coefficient (K_{inst}) of both surrogate HVO and ammonia fuels were analyzed. The effect of initial droplet temperature was examined by changing the coolant temperature in this study, and the droplet temperature during evaporation is also discussed. Figure 5 reveals that HVO surrogate fuels exhibit shorter droplet lifetimes and higher evaporation rates than diesel under all ambient conditions due to their lower density, surface tension, and boiling point. Among HVO surrogate fuels, HVO:C_{15}-C_{18}/isododecane has the shortest droplet lifetimes because adding iso-dodecane reduces the initial heating period due to a lower boiling point. Moreover, it was found that the evaporation characteristics are affected by not only the boiling point but also fuel compositions and thermodynamic properties such as thermal conductivity, latent heat of vaporization, and specific heat of gas. Increasing temperature decreases droplet lifetime and increases the evaporation rate due to high heat transfer from the ambient gas. However, the effect of pressure on droplet lifetime relies on ambient temperature (T_{amb}). As pressure increases, droplet lifetime increases at $T_{amb} < T_c$ (critical temperature) and decreases at $T_{amb} > T_c$. Increasing pressure at $T_{amb} \sim T_c$ has no significant effect on droplet lifetime.



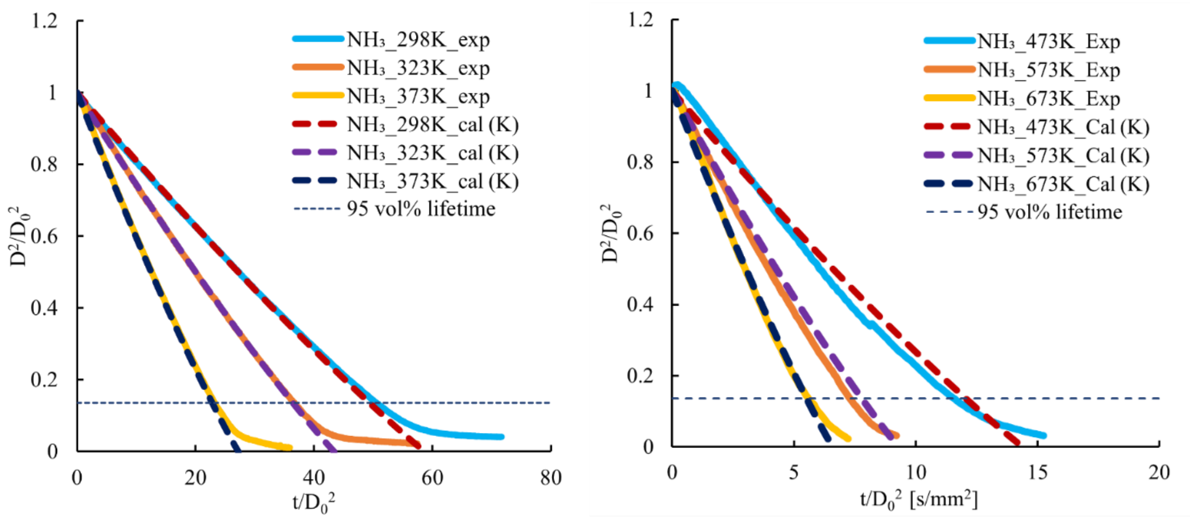
(a) 573K



(b) 873K

Figure 5 Histories of normalized D^2 for HVOs and diesel fuel at (a) 573K and (b) 873K.

Ammonia's low density, surface tension, and boiling point favor evaporation, while high vapor pressure and latent heat of vaporization can significantly influence evaporation behavior. History of normalized D^2 for ammonia is shown in Figure 6. The normalized diameter squared (D^2/D_0^2) decreases linearly, following the D^2 law, with deviations at later stages of evaporation while the K_{inst} decreases over time. This is due to the effect of impurities and changes in heat and mass transfer around the droplet. Due to its polarity, ammonia can attract and absorb moisture, which can impact the rate of evaporation. Increasing ambient temperature reduces droplet lifetime and enhances the evaporation rate due to the enhanced heat transfer from the ambient gas while initial droplet temperature has a minor effect on evaporation and is not the primary factor. Instead, other factors like ambient temperature and pressure play a more significant role in controlling the overall evaporation rate. Droplet temperature measurements show an initial rapid temperature drop due to the evaporative cooling effect from the latent heat of vaporization. Throughout evaporation, droplet temperature remains relatively stable under tested conditions, indicating a thermal balance between heat transfer from the ambient gas and heat used for vaporization. The theoretical model incorporating natural convection aligns closely with experimental results, highlighting the critical role of buoyancy-induced flows in enhancing ammonia droplet evaporation.



(a) (b)

Figure 6 History of normalized D^2 for ammonia during the whole evaporation process at P_{amb} = 0.95 MPa and $T_{coolant}$ = -25℃. Experiment vs calculation with natural convection *(K)*

In conclusion, HVO fuels evaporate faster than diesel due to lower density, surface tension, and boiling point. HVO:C_{15}-C_{18}/isododecane shortest droplet lifetime due to isododecane's low boiling point. Evaporation depends on boiling point, fuel composition thermal properties. Pressure effect on evaporation relies on temperature. $T_{amb} < T_c$: Higher pressure reduces evaporation. $T_{amb} > T_c$: Higher pressure increases evaporation. $T_{amb} \sim T_c$: Pressure has minimal impact. For ammonia, the experimental setup is capable of conducting droplet evaporation experiments under various conditions. Low density, boiling point, and high vapor pressure enhance evaporation while high latent heat causes a cooling effect. The evaporation rate decreases over time due to reduced natural convection. Natura convection (Buoyancy-induced flow) is significant in accurately capturing ammonia droplet evaporation. These findings hold significance for optimizing fuel injection strategies, enhancing combustion efficiency, and developing comprehensive evaporation models.