

#### MATHEMATICAL MODELLING OF ENGINEERING PROBLEMS

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## Effect of ambient conditions on n-heptane droplet evaporation

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### ABSTRACT

Based on the theory of heat and mass transfer, an evaporation model for single droplet in the convection heat air environment was established. By comparing the experimental data, the correctness of the model was verified. The effects of the initial droplet diameter, ambient temperature, ambient pressure and flow intensity on the n-heptane droplet evaporation characteristics was analyzed. The results showed that ambient temperature, ambient pressure and flow intensity has a great influence on the n-heptane droplet evaporation, and the ambient temperature is the main factor, when the ambient temperature increased from 400K to 600K, the droplet lifetime decreased from 44ms to 6.5ms, shortened by 85.23%. Ambient temperature and flow intensity can accelerate n-heptane droplet evaporation, but the evaporation time was extended with the increase of the ambient pressure.

Keywords: Evaporation, Single Droplet, N-Heptane, Ambient Pressure, Flow Intensity.

#### **1. INTRODUCTION**

Droplet evaporation is very common in the power plants, such as gas turbine, steam turbine and internal combustion engine. The evaporation process of liquid droplets in an internal combustion engine cylinder can be studied by a single droplet evaporation. Study single droplet evaporation process plays an important role in the process of spray and combustion [1].

At present, there are two research methods to study single droplet evaporation, namely, experimental research and theoretical research. In the experimental study, the liquid droplet can be placed in a high temperature environment by means of the quartz wire suspension and acoustic levitation method, the droplet evaporation characteristics can use a high-speed camera take photos to study. However, the experimental methods are complicated and the current technical conditions are difficult to study the evaporation of liquid droplets under high pressure and high convective environment. By establish the theoretical model, theoretically study the evaporation characteristics of single droplet can make up for the deficiency of the experiment. HU Peng.et al researched the n-heptane single droplet evaporation characteristic in a CO2-water vapor environment. The results show that with the increase of ambient pressure, ambient temperature, the ignition delay and droplet lifetime were all shortened. The influence of ambient temperature on nheptane droplet evaporation is greater [2]. DING Jixian.et al studied the effects of pressure convection environment on droplet evaporation characteristics by establish a n-heptane single droplet evaporation model in nitrogen atmosphere. The results show that in high temperature and strong convection environment, increasing the ambient pressure can promote the droplet evaporation, but in low temperature and weak convection environment, increasing the ambient pressure can delay droplet evaporation [3]. From the literature, n-heptane droplet evaporation characteristics under high temperature and high pressure atmosphere are different from the conditions above all, there are few studies on droplet evaporation at high pressure and high temperature conditions. Therefore, it is necessary to study the n-heptane droplet evaporation characteristics under high temperature and high pressure atmosphere.

In this paper, based on the theory of heat and mass transfer, an evaporation model for single n-heptane droplet under the convection heat air environment was established. The model can be used to calculate the droplet diameter variations during evaporation, then it can analyze evaporation characteristics. By comparing the experimental data, the correctness of the model is verified. The influence of the initial droplet diameter, ambient temperature, ambient pressure and flow intensity on n-heptane droplet evaporation characteristics were analyzed.

#### 2. CLACULATION METHOD

#### 2.1 Evaporation model

The droplet evaporation process is a very complex process, in order to facilitate calculation, the evaporation model is set up based on the following assumptions: (1) the droplet is spherically symmetric; (2) There is no temperature gradient inside the liquid droplet, and the temperature and composition in the space are evenly distributed; (3) The physical properties in space is uniform distribution, and Le=1.

Based on the above assumptions, establish energy conservation, mass conservation, and component conservation equations for a single droplet, the evaporation rate is calculated as follows [4]:

$$\dot{m} = \frac{\pi Dk}{C_p} N u \ln(1 + B_M)$$
<sup>(1)</sup>

$$B_M = \frac{Y_s - Y_\infty}{1 - Y_s} \tag{2}$$

$$Y_s = \frac{x_s M}{x_s M + M_{air} (1 - x_s)} \tag{3}$$

$$x_s = x \frac{P_{sat}}{P} \tag{4}$$

The flow velocity will lead to forced convection, the impact through the correction of Nu to consider.

$$Nu = 2 + (Nu_0 - 2) / F(B_M)$$
(5)

$$F(B_M) = (1 + B_M)^{0.7} \frac{\ln(1 + B_M)}{B_M}$$
(6)

$$Nu_0 = 2 + 0.552 \,\mathrm{Re}^{0.5} \,\mathrm{Pr}^{1/3} \tag{7}$$

$$Re = \frac{\rho_{\infty}DU}{\mu_m}$$
(8)

$$\Pr = \frac{C_p \mu_m}{k} \tag{9}$$

The droplet evaporation rate is the function of temperature, therefore droplet evaporation rate can be expressed by

$$\dot{m} = 4\pi r^2 \rho_m \frac{dr}{dt} \tag{10}$$

The droplet mass flow is equal to the rate of droplet evaporation, combined with equation (1) and (10), Droplet diameter is expressed by

$$\frac{dD}{dt} = -\frac{2k}{C_p D \rho_m} N u \ln(1 + B_M)$$
(11)

t=0,  $D=D_0$ , integrate formula (10), we obtained D is

$$D = \sqrt{D_0^2 - \frac{4k}{C_p \rho_m} N u \ln(1 + B_M) \Delta t}$$
(12)

# 2.2 Thermal physical properties of liquid droplets and ambient gas mixtures

The n-heptane droplet specific heat capacity is given by the formula (13) [5]:

$$C_{p} = 2.25 \times 10^{3} + 1.11 \times 10^{3} \tilde{T} + 1.87 \times 10^{3} \tilde{T}^{2}$$

$$-4.89 \times 10^{3} \tilde{T}^{3} + 5.16 \times 10^{3} \tilde{T}^{4}$$
(13)

The saturated vapor pressure of n-heptane is given by the formula (14) [6]:

$$P_{sat} = (0.082 + 1.078\tilde{T} + 8.707\tilde{T}^{2} + 11.03\tilde{T}^{3} + 64.967\tilde{T}^{4} - 40.802\tilde{T}^{5} + 7.74\tilde{T}^{6}) \times 10^{5}$$
(14)

Liquid density is given by the formula (15), (16) [5]:

$$T < 0.793$$

$$\rho_m = 678.93 - 248.73\tilde{T} - 251.16\tilde{T}^2 + 735.16\tilde{T}^3 - (15)$$

$$882.37\tilde{T}^4$$

$$T > 0.793$$

$$\rho_m = -3.16 \times 10^5 + 8.04 \times 10^5 \tilde{T} - 5.10 \times 10^5 \tilde{T}^2 \qquad (16)$$

The viscosity of n-heptane is given by formula (17) [6]:

$$\mu_m = \left(\frac{1}{1.53 + \frac{T - 20}{233}}\right)^{3.758} + 273.15 \tag{17}$$

The thermal conductivity is calculated by formula (18) :

$$k = 0.122 - 0.137T \tag{18}$$

where 
$$\tilde{T}$$
 is normalized temperature,  $\tilde{T} = \frac{T - T_0}{T_0}$ 

Binary diffusion coefficient is calculated by formula (19):

$$D_m = \frac{0.00143T^{1.75}}{pM_{AB}^{0.5}[(\Sigma_v)_A^{1/3} + (\Sigma_v)_B^{1/3}]^2}$$
(19)

where  $M_{AB} = 2(\frac{1}{M_A} + \frac{1}{M_B})^2$ ,  $\Sigma_v$  is atomic diffusion volume.

#### 2.3 Model validation

In this section, the evaporation model is validated against the experimental data reported in Daif .et al [7]. In the experiment, the ambient temperature is 294K, the initial droplet diameter is 1.386mm, the initial droplet initial temperature is 290K, the ambient pressure is 0.1MPa, the air flow intensity is 0m/s.

Fig. 1 shows the experimental values and calculated values of n-heptane droplet evaporation. It is clearly to see, the calculated values is agree with experimental values very well. Therefore, the model can analyze the evaporation characteristics of n-heptane droplet evaporation.



**Figure 1.** The experiment and calculated value of n-heptane droplet evaporation under normal temperature and pressure

#### **3. RESULTS AND DISCUSSION**

#### 3.1 The effect of initial droplet diameter

Under ambient temperature T=400K, ambient pressure p=1MPa, flow intensity U=1m/s and initial droplet temperature 300*K*, the evaporation characteristics of different initial diameter (0.8mm, 0.9mm and 1.0mm) was calculated. And the effect of initial droplet diameter on n-heptane droplet evaporation was studied.

Fig. 2 given the variation of droplet diameter with different initial droplet diameter (0.8*mm*,0.9*mm* and 1.0*mm*).

Under the same ambient condition, the droplet lifetime increases with increasing the initial diameter. When the droplet diameter decrease from 1.0mm to 0.9mm, 0.8mm, the droplet lifetime decreasing from 61ms to 52ms,44ms, shortened by 14.75%, 27.86%, respectively. This is because droplet in a high ambient temperature environment, bigger droplet will need the longer response time rise to the ambient temperature under the same state.

#### 3.2 The effect of ambient temperature

In this section, droplet diameter is 0.8mm, ambient pressure p=1MPa, flow intensity U=1m/s and initial droplet temperature 300*K*, the evaporation characteristics of different ambient temperature (400*K*,500*K* and 600*K*) was calculated. And the effect of ambient temperature on n-heptane droplet evaporation was studied.



Figure 2. Time variations of droplet diameter with different initial droplet diameter

It can be seen from fig. 3 droplet lifetime decreases with increasing the ambient temperature. When the ambient temperature increase from 400K to 500K, 600K, the droplet lifetime decreasing from 44ms to 33.5ms, 6.5ms, shortened by 23.86%, 85.23%, respectively. The temperature rises from 500K to 600K, the droplet evaporation time decreases sharply, which is very different from the situation of ambient temperature increase from 400K to 500K. This is because under high temperature, the physical properties of fuel changed dramatically, which led to the severely increase of evaporation rate. And this conclusion agrees with the conclusion in [2].



Figure 3. Time variations of droplet diameter with different ambient temperature

#### 3.3 The effect of ambient pressure

In this section, droplet diameter is 0.8mm, ambient temperature T=400K, flow intensity U=1m/s and initial droplet temperature 300K, the evaporation characteristics of different ambient pressure (1MPa, 2MPa and 3MPa) was calculated. And the effect of ambient pressure on n-heptane droplet evaporation was studied.

In fig. 4. n-heptane droplet evaporation rate increases with the decreasing the ambient, this is consistent with the results of many experiments and conclusions [2-4]. When the ambient pressure increase from 1MPa to 2MPa, 3MPa, the droplet lifetime increased from 44ms to 50ms, 55ms. It can be seen from fig. 5. diffusion coefficient is inversely proportional to ambient pressure, high ambient pressure will lead to small diffusion coefficient, and the low evaporation rate of droplets.



Figure 4. Time variations of droplet diameter with different ambient pressure



Figure 5. Temperature variations of diffusion coefficient with different ambient pressure

#### 3.4 The effect of flow intensity

By changing the velocity of air movement, the influence of the flow intensity on the droplet evaporation characteristics can be simulated. In this section, droplet diameter is 0.8mm, ambient pressure p=1MPa, ambient temperature T=400K and initial droplet temperature 300K, the evaporation characteristics of different flow intensity (1m/s, 2m/s) and 3m/s) was calculated. And the effect of flow intensity on nheptane droplet evaporation was studied.



Figure 6. Time variations of droplet diameter with different flow intensity

Fig. 6 represent the time variations of droplet diameter with different flow intensity. It is clearly to see high flow intensity will accelerate droplet evaporation. When the flow intensity increase from 1m/s to 2m/s, 3m/s, the droplet lifetime decreased from 44ms to 30.5ms and 25ms, shortened

by 30.68%, 43.18%, respectively. Therefore, air movement accelerated the evaporation process of the droplet.

## 4. CONCLUSION

1. Based on the theory of heat and mass transfer, an evaporation model for single droplet in the convection heat air environment was established. By comparing the experimental data, the correctness of the model is verified.

2. Ambient temperature, ambient pressure and flow intensity has a great influence on the n-heptane droplet evaporation, and the ambient temperature is the main factor. Ambient temperature and flow intensity can accelerate n-heptane droplet evaporation, but with the increase of ambient pressure, the droplet evaporation time becomes longer.

3. In droplet evaporation process, when the ambient temperature increased from 400K to 600K, the droplet lifetime decreased from 44ms to 6.5ms, shortened by 85.23%. When the ambient pressure increase from 1MPa to 3MPa, the droplet lifetime increased from 44ms to 55ms. When the flow intensity increase from 1m/s to 3m/s, the droplet lifetime decreased from 44ms to 25ms, shortened by 43.18%.

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Spalding mass transfer number

Specific heat capacity

Diffusion coefficient

Thermal conductivity

Droplet diameter

Molar mass

pressure

Lewis number Nu Nusselt number

## NOMENCLATURE

BM

Dm

k

М

Le

Р

C D

Pr	Prandtl number
r	Droplet radius
U	Velocity
х	Molar fraction
Y	Mass fraction

## Greek symbols

Viscosity
Density

## Subscripts

S	Surface
$\infty$	Infinite
sat	Saturated
0	Initial value