Numerical investigation on evaporation characteristics of kerosene droplets with dilute concentrations of aluminum nanoparticles at elevated temperatures

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Abstract. We have numerically investigated the problem of kerosene droplets evaporation with dilute concentrations of aluminum nanoparticles at elevated temperatures. The aim of the research was to develop a mathematical model describing the evaporation process and obtain numerical simulation data which is in good agreement with an experimental data. The dependences of kerosene droplet evaporation time on its initial diameter and ambient temperature are presented in this paper.

1. Introduction

Combustion of liquid fuels is a very complex process consisting of several stages. In most cases liquid fuel is atomized thus it consists of small particles in the form of droplets. Combustion of liquid fuels always occurs in the vapor phase therefore the evaporation process always precedes the process of drop burning. The drop placed in a high-temperature environment is surrounded by its vapors that create a spherical zone around it. In the case of steady state of combustion around the droplet, the droplet burning rate depends on the evaporation rate. The thickness of the evaporation zone depends on the ambient temperature and on the evaporation parameters of the fuel: the higher the ambient temperature, the greater the thickness of the evaporation zone. The evaporation zone also increases with decreasing the boiling point and the heat of fuel evaporation.

A nanosized aluminum powder is added in kerosene drops to intensify the evaporation process [1]. The results of an experimental study on evaporation characteristics of kerosene droplets containing small concentrations (0.1%, 0.5%, and 1.0% by mass) of aluminum nanoparticles at different ambient temperatures and normal pressure are presented in [1]. The experiments were performed with an isolated nanofluid fuel droplet suspended by a fine SiC fiber (100 $\mu$m diameter). The heat loss from the fiber was neglected during most of a droplet’s lifetime. The initial average diameter of a droplet was $1.0 \pm 0.10$ mm. The ambient temperature was varied from 400 to 800°C, which is higher than the boiling point of kerosene and the melting point of the Al nanoparticles, and the ambient pressure was kept constant at 0.1 MPa. High-temperature ambience was provided by a freely falling electric furnace. A flexible image-processing code was developed using Matlab to obtain the droplets’ diameters from the captured images. This code was executed iteratively for each image, resulting in the temporal variation of the droplet diameter during evaporation. The droplet evaporation rate was
obtained from the temporal history of the droplet diameter squared by measuring the slope of its linear regression.

This paper is devoted to the mathematical modeling of kerosene drop evaporation in a high-temperature ambient. The aim of the work is to develop a mathematical description of the droplet evaporation process at elevated temperatures and to perform a calculation and theoretical analysis of the process by the comparison the calculation results and experimental data.

2. Mathematical model

The mathematical model is constructed under the assumptions from [2]: a kerosene drop is put in an inert high temperature ambient (nitrogen) at atmospheric pressure. The drop heats up and evaporates. The temperature distribution in the drop is uniform. The heat expansion of the drop is neglected. The ambient temperature is assumed to be constant. The heat exchange between the drop and the surrounding medium is provided by convection and radiation. The convective heat transfer of the drop with the surrounding gas is described by Newton's law for heat exchange with a heat transfer coefficient taking into account the Stefan flow of kerosene vapor from the droplet surface [3]. Radiant heat exchange is described by the Stefan-Boltzmann law. The heat supplied to the drop from the environment is spent on heating kerosene drop from the initial temperature to the boiling point and on partial evaporation. After reaching the boiling point all heat supplied to the drop is expended on its evaporation. It is assumed that a certain amount of nanosized aluminum powder added to kerosene changes the emissivity factor of the drop.

The equation system describing the heating up and evaporation processes of the drop under the made assumption has the following form:

At \( T < T_{\text{boiling}} \):

\[
c_d \rho_d V \frac{dT}{dt} = -\alpha(T - T_\infty)S - \sigma \varepsilon (T^4 - T_\infty^4)S + L \rho_d \frac{dV}{dt},
\]

\[
\rho_d \frac{dV}{dt} = -\beta(\rho_v - \rho_s)S.
\]

At \( T = T_{\text{boiling}} \):

\[
L \rho_d \frac{dV}{dt} = \alpha(T - T_\infty)S + \sigma \varepsilon (T^4 - T_\infty^4)S.
\]

The initial condition:

\[
V(0) = V_0, \quad T(0) = T_0,
\]

where \( c_d \) is the droplet specific heat; \( \rho_d \) is the kerosene density; \( V \) is the droplet volume; \( S \) is the droplet surface area; \( t \) is time; \( \alpha \) is the heat transfer coefficient; \( \sigma \) is the Stefan-Boltzmann constant, \( \varepsilon \) is the emissivity factor; \( \beta \) is the mass-transfer coefficient; \( T \) is the droplet temperature; \( T_\infty \) is the ambient temperature infinitely far from the droplet; \( T_{\text{boiling}} \) is kerosene boiling temperature; \( L \) is the evaporation heat; \( \rho_v \) is density of saturated kerosene vapor; \( \rho_s \) is density of kerosene vapor infinitely far from the droplet.

To determine \( \alpha \) and \( \beta \), we use the Nusselt number. The Stefan flow dependence for the droplet [3] is

\[
Nu_w = \frac{\alpha r_d(t)}{\lambda_d} = \frac{r_d(t) w/a}{\exp(r_d(t) w/a) - 1},
\]
where \( r_d \) is the droplet radius; \( \lambda_g \) is the gas thermal conductivity coefficient; \( w \) is velocity of the kerosene vapor flowing off the droplet surface; \( a = \lambda_g / (c_g \rho_g) \) is gas thermal diffusivity; \( c_g \) is gas specific heat around the droplet; \( \rho_g \) is gas density around the droplet.

The Stefan flow velocity is defined from the mass conservation law:

\[
\rho_d \frac{dV}{dt} = -\rho_g w S ,
\]

then

\[
w = \frac{\rho_d}{\rho_g} \frac{dr_g}{dt} , \quad \alpha = \frac{Nu_w \lambda_g}{r_g(t)} .
\]

To obtain the mass-transfer coefficient \( \beta \), we use the analogy of the heat exchange and mass transfer processes. The intensity of mass transfer is determined by the Sherwood number \( Sh = \beta r_g(t)/D \), where \( D \) is the diffusion coefficient. Taking for the gas the Lewis number \( Le = D / (\lambda_g / c_g \rho_g) = 1 \) and the equality \( Sh_w = Nu_w \), we obtain:

\[
\beta = \frac{DSh_w}{r_g(t)} = \frac{\lambda_g Nu_w}{c_g \rho_g r_g(t)} ,
\]

\[
\lambda_g = \lambda_0 \sqrt{(T/T_0)}^2 .
\]

The density of saturated kerosene vapor is determined by the Clausius–Clapeyron relation

\[
p = Ae^{-L/RT} ,
\]

where \( p \) is the saturated vapor pressure, \( L \) is the specific heat of evaporation, \( R \) is the universal gas constant, and \( A \) is a constant. The value \( A \) is determined from the known boiling point \( T_{\text{boiling}} \) at a pre-set pressure \( p_a \). Applying the ideal gas equation for a known temperature and the pressure of saturated vapor we can find the density of saturated vapor at the surface of the drop:

\[
\rho_{sv} = \frac{p}{RT} e^{-L/RT} .
\]

To determine the similarity parameters for the drop evaporation, we write the system of equations (1) - (3) in dimensionless variables. The following quantities were chosen as scales: \( r_0 \) is the spatial scale (the initial droplet radius); \( T_0 \) is the temperature scale (the initial droplet temperature); \( \rho_d \) is density scale (the liquid kerosene density); \( t_0 = \frac{c_d \rho_d r_0^2}{\lambda_0} \) is the time scale. The dimensionless variables are

\[
\bar{\tau} = \frac{r}{r_0} , \quad \theta = \frac{T}{T_0} , \quad \tau = \frac{t}{t_0} , \quad \bar{\rho} = \frac{\rho}{\rho_d} , \quad \bar{w} = \frac{w}{r_0/t_0} .
\]

At \( \theta < \theta_{\text{boiling}} \):

\[
\frac{\bar{\tau}^2}{3} \frac{d\theta}{d\tau} = -\theta^{2/3} \left( \theta - \theta_{eq} \right) Nu_w - \bar{\rho} \left( \bar{\theta}^4 - \theta_{eq}^4 \right) + \frac{\bar{T}}{2} \frac{d\bar{T}}{d\tau} ,
\]

\[
\frac{d\bar{T}}{d\tau} = -C_g \frac{\theta^{2/3}}{\rho_g} \left( \bar{\theta}_{sv} - \bar{\theta}_{eq} \right) Nu_w .
\]
At $\theta = \theta_{\text{boiling}}$:

$$\frac{\bar{L}}{2} \frac{d\bar{r}^2}{d\tau} = \theta^{2/3} (\theta - \theta_e) \text{Nu}_w + P\overline{\text{Pr}} (\theta^2 - \theta_e^2).$$  \hspace{1cm} (11)

The initial conditions:

$$\bar{r}(0) = 1, \quad \theta(0) = 1.$$ \hspace{1cm} (12)

$$\text{Nu}_w = \frac{\bar{r} (\tau) \overline{\rho}_w / \theta^{2/3} C}{\exp(\bar{r} (\tau) \overline{\rho}_w / \theta^{2/3} C) - 1},$$ \hspace{1cm} (13)

$$\overline{\omega} = - \frac{1}{\overline{\rho}_w (\tau)} \frac{d\overline{\rho}}{d\tau}.$$ \hspace{1cm} (14)

The dimensionless parameters appeared in the equation system (9) - (11) are the following: $P = \sigma a T_0^4 / \lambda_0$ characterizes the radiation heat transfer, $\bar{L} = L / (T_0 c_d)$ characterizes the evaporation heat, $C = c_d / c_g$ is the liquid and gas specific heat ratio.

Under $P = 0$ the solution of the equation system (9)-(11) depends on values $\bar{L}$ and $C$. Therefore the solution can be presented as a function $\frac{\bar{r}^2}{t_0} \left( \frac{t}{d_0^2} \right)$ [1]. However under $P \neq 0$ the solution cannot be presented in the mentioned form.

### 3. Results and discussion

The equation system (1) – (3) with initial conditions (4) and expressions (5) – (8) was solved by the Euler method. The values of thermophysical quantities for the calculations were taken as follows: $\rho_d = 800 \text{ kg/m}^3$, $c_d = 2.2 \text{ kJ/(kg \cdot K)}$, $L = 222 \text{ kJ/kg}$, $\lambda_0 = 0.017 \text{ W/(m \cdot K)}$, $T_{\text{boiling}} = 175 \text{ °C}$, $T_0 = 25 \text{ °C}$, $R = 8.314 \text{ J/(mol \cdot K)}$, kerosene molar mass $0.099 \text{ kg/mol}$, $p_a = 101235 \text{ Pa}$, $\rho_e = 0$, the ambient temperature $T_\infty$ was in the range 400–600 °C, the droplet diameter was equal to $d_0 = 1.0 \text{ mm}$.

To match the calculated evaporation time of a pure kerosene droplet with experimental one we varied the value $\varepsilon$. Figure 1a shows the results of the calculated and experimental data from [1] on the evaporation dynamics of a pure kerosene droplet in time. The results are presented in the form of $\frac{d^2}{d_0^2} \left( \frac{t}{d_0^2} \right)$ as in [1, 4]. The calculated and experimental time intervals of droplet evaporation are in good agreement under $\varepsilon = 0.88$. During this time interval 90% of the initial droplet mass evaporates. The dynamics of the droplet size change in time also coincides well with the results of experimental measurements (figure. 1a) [1]. Figure 1b provides the results on experimental and calculation data of the kerosene droplet evaporation dynamics with the addition of 1% (by mass) of a nanosized aluminum powder. The calculation is carried out at $\varepsilon = 0.95$. The obtained results are also in good agreement with the results of experimental data [1]. The presence of a nanosized aluminum powder in a kerosene droplet increases the drop heat absorptivity which reduces the time of its evaporation.

Figure 2 presents the calculation results on the dynamics of the kerosene droplet size change in time for different values of the initial droplet diameter. Solid lines are plotted for pure kerosene droplets, dashed lines are for droplets containing 1% aluminum nanopowder. The ambient gas temperature is 500°C.
4. Conclusions
We have presented a mathematical model of the kerosene drop evaporation process in an inert gas at high ambient temperature. The model takes into account conductive and radiant heat exchange of a drop with gas and the influence of the kerosene vapor Stefan flow on the intensity of heat transfer. The effect of dilute concentration of aluminum nanoparticles in kerosene droplet on the evaporation rate is taken into account by of the emissivity factor of the drop. The dependences of the dynamics of the kerosene droplet diameter change in time are obtained which are in good agreement with experimental data from [1]. The calculation results shows that due to the radiation heat transfer the droplet evaporation time is not proportional to the square of its initial diameter.

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References

[1] Javed I, Baek S W, Waheed K, Ali G and Cho S O 2013 Combust. Flame 160(12) 2955–63
[2] Kozlov E A and Krainov A Yu 1999 Combust. Explos. Shock Waves 35(6) 15–21
[3] Nigmatulin R I 1990 Dynamics of Multiphase Media (CRC Press; Rev Sub edition)
[4] Turns S R 2006 An Introduction to Combustion: Concepts and Applications (McGraw-Hill Science)