Flame Characteristics of a n-octane Droplet under Electrical Field

Kiyotaka YAMASHITA\textsuperscript{1}, Osamu IMAMURA\textsuperscript{1}, Jun OSAKA\textsuperscript{2}, Shinji NAKAYA\textsuperscript{3}, Mitsuhiro TSUE\textsuperscript{1} and Michikata KONO\textsuperscript{1}

\textsuperscript{1} The University of Tokyo, Tokyo, Japan, tt57061@mail.ecc.u-tokyo.ac.jp
\textsuperscript{2} Nagoya University, Nagoya, Japan
\textsuperscript{3} Osaka Prefecture University, Osaka, Japan

Abstract
Normal-octane droplet fuel combustion under uniform electrical field is investigated by using experimental and numerical method. The flame properties including the deformation of flame shape and burning velocity is measured from captured flame pictures. In order to reveal the mechanism of deformation and combustion enhancement under electrical field the numerical prediction which includes the soot particle effect is implemented. The changes of deformation ratio and increasing of burning rate constant are obtained comparing the droplet flame with no applied voltage and 4kV case. Although the numerical results are underestimated than experimental results because of no consideration of soot formation, enhancement of vaporizing is shown in numerical predictions. The profiles of Coulomb force, charge density, electrical field and ion species are also simulated. Local increasing of momentum with electrical field changing is shown from results. The profile of charge density which is depending on ion species is considered and deformation mechanism is revealed. It is seen that the movement of flame under uniform electrical field caused the increasing of inlet heat into the surface of droplet, so then vaporizing of droplet is enhanced.

1. Introduction
Flame characteristics with electrical field are investigated. Deformation of flame, promotion of combustion and suppression of soot production are reported in past studies\textsuperscript{1,2}. But almost about this phenomenon is researched by experimental method. With high voltage, there are many disturbances and it is difficult to measure some informations of flame. On the other hand, numerical prediction of this phenomenon is hardly carried out in past. Some simple calculation model or only chemical kinetics analyses are reported\textsuperscript{3,4}. It is thought that numerical simulation is needed to reveal the phenomenon. From these backgrounds authors conducted experimental and numerical simulation of hydrocarbon combustion under electrical field. By these researches the temperature or flow field changes of flame is investigated in 1-D or 2-D flames\textsuperscript{5,6}. But the sooting flame like heptane or octane fuel is different from non-sooting flame like ethanol fuel. It is said that the soot particles can be electrical charged and effect on the flow field in flam. So then the sooting flame is studied by n-octane flame with uniform electrical field.

2. Experiments
All experiments are carried out under microgravity environment which is obtained using a drop tower in Fig. 1. Height of the tower is about 10m and the obtained microgravity time is about 0.8sec. A drop box is dropped from top of the tower and stopped in the buffer at bottom. All combustion experiment and measurement are implemented during the box is dropping. The drop box is shown in Fig. 1. It includes the fuel supply system, optical system, control system and combustion chamber. The combustion chamber is shown in Fig. 1. It includes fuel supply needle, fuel pomp, two flat electrodes, hot wire and suspended line. The procedure of experimental is including:

1. The liquid fuel is supplied using a fuel pump and needle. The fuel is suspended at the edge of the line.
2. Electrical voltage is applied between two flat electrodes.
3. Suspended wire above the drop box is cut and dropping is started.
4. Just after dropping is started, hot wire is turned on electricity and its body is heated immediately.
5. Fuel droplet is ignited by the hot wire and combustion is continued until the box is stopped.
6. The movie of fuel droplet and flame is captured and it is stored in a PC.

The change in flame shape is measured using captured flame shape pictures. The burning rate constant is defined using the change velocity in droplet diameter like eq. (1).\textsuperscript{7}
\[ K = \frac{d(d_i)^2}{dt} \]  

3. Simulations

A numerical simulation which includes the droplet combustion, vaporizing, electrical fields and soot movement is carried out. The governmental equations are including:

\textbf{(Mass conservation)}

\[ \frac{\partial \rho}{\partial t} + \text{div}(\rho u) = 0 \]  

\textbf{(Momentum conservation)}

\[ \frac{\partial (\rho u)}{\partial t} + \text{div}(\rho uu) = \text{div}(\rho \text{grad}u) - \text{grad}\rho + B_s \]  

\textbf{(Energy conservation)}

\[ \frac{\partial (\rho H)}{\partial t} + \text{div}(\rho uu) = \text{div}(\lambda \text{grad}T) + \frac{\partial \rho}{\partial t} + u \cdot \text{grad}\rho + \phi + Q \]  

\textbf{(Species conservation)}

\[ \frac{\partial (\rho Y)}{\partial t} + \text{div}(\rho Y - \rho D \text{grad}Y) = R_s \]  

\textbf{(Charge conservation)}

\[ q = (n^+ + n^-)e \]  

(Relation of electrical field and potential)

\[ \text{grad}V = -E \]  

(Relation of electrical potential and charge density)

\[ \text{div}E = \frac{\Sigma \rho Y q_i}{\epsilon_0} \]  

(Relation of body force and electrical field)

\[ B_{\text{bou}} = qE \]  

(Relation of drift velocity and electrical field)

\[ u_{\text{add}} = \mu E \]  

(Gas Properties)

- Gas density

\[ \rho = \sum_{i=1}^{K} \rho_i \]  

- Gas specific heat

\[ c_p = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \]  

- Gas viscosity

\[ \eta_s = \frac{5}{16} \sqrt{\frac{m_i k_s T}{\pi \sigma_i^2 \Omega^{(2/3)}}} \]  

(Liquid Properties)

- Liquid density

\[ \rho = A \cdot B^{-0.7 - 0.3 X} \]  

- Liquid specific heat

\[ c_p = b_1 + b_2 T + b_3 T^2 + b_4 T^3 \]  

- Liquid thermal conductivity

\[ \lambda_i = c_1 + c_2 T + c_3 T^2 \]  

- Gas counter diffusion coefficients

\[ D_{\text{bou}} = 0.0006280 \sqrt{\frac{1}{\Omega^{(1/3)}}} \]  

Fig. 1 Drop tower, drop box and combustion chamber
Boundary Conditions

- Mass conservation boundary conditions

\[
\rho \left( \frac{dR}{dt} \right) = \rho \left( \frac{dR}{dt} \right)
\]

- Species conservation boundary conditions

\[
\rho \left[ Y \left( \frac{dR}{dt} \right) - D \left( \frac{\partial Y}{\partial r} \right) \right] = \rho \left[ Y \left( \frac{dR}{dt} \right) - D \left( \frac{\partial Y}{\partial r} \right) \right]
\]

Conservation equations include fluid (2) (3), thermal (4), species (5) and electrical charge (6). An effect of electrical field on flow field is considered using eq. (9). The Coulomb force \( \mathbf{B} \) is added to the momentum equations (2), (3) as the body force. Electrical potential \( \mathbf{V} \) is calculated using eq. (7). Electrical field strength is calculated from charge density using eq. (8). The effect of variable electrical field strength is reported in the past study. \( \rho \) The drift velocity from the electrical field is added to the velocity of the both positive ion and electron using eq. (10).

Calculation field is shown in Fig. 2. The fuel droplet is set on the center of the field. Two plate electrodes are set both side of droplet and the distance between electrodes is 5cm. Although the phenomenon is occurred in the 3D space, the calculation is carried out in the 2D field because the field has symmetry shape with X-X' axis. Further more the shape and area of electrodes are inconsequential, the area of electrodes are assumed infinity. The mesh is set crossing both electrodes and surface of droplet.

Calculation method and condition is shown in Table 1. Reaction mechanisms are composed from 150 chemical species reactions and 10 ion species reactions. Chemical species reaction equations are obtained as the result of reducing of about 1000 n-octane elementary equations. \( \rho \) Ion species equations are reduced from 50 elementary equations. \( \rho \) Mobility of ion particle is given from past studies. \( \rho \) Gas initial condition is room temperature, atmospheric pressure. Liquid fuel is also room temperature and pure n-octane. Ignition is carried out using a high temperature ambient gas.

Some assumptions are adopted to save the calculate time. It is following:

1. The gravity force is not considered to remove the effects of natural convection.
2. The droplet diameter is decreasing virtually for the calculation of the burning rate constant. (The position of droplet surface does not move.)
3. Flat electrodes have infinity area.
4. Increase of energy, induced magnetic field by electrical fields and radiation are ignored.

Soot is considered as isothermal and non vaporizing particle. Just momentum is exported with gas phase. In this calculation, the momentum conservation of solid phase is calculated using following equation:

\[
m \frac{\partial U}{\partial t} = D \left( U_s - U_s \right) - V_p \nabla p
\]

The interface source between gas phase and solid phase is calculated using following equation:

<table>
<thead>
<tr>
<th>Method</th>
<th>Spatial Finite Volume Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temporal</td>
<td>Implicit method (1st order)</td>
</tr>
<tr>
<td>Iteration</td>
<td>Simplest method</td>
</tr>
<tr>
<td>Mesh</td>
<td>Body fitted coordinate</td>
</tr>
<tr>
<td>Coordinate</td>
<td>2-D ( \xi - \eta )</td>
</tr>
<tr>
<td>Division</td>
<td>( \xi:40, \eta:40 )</td>
</tr>
<tr>
<td>Number</td>
<td>1600</td>
</tr>
<tr>
<td>Reaction</td>
<td>150 equations</td>
</tr>
<tr>
<td>Ion</td>
<td>10 equations</td>
</tr>
<tr>
<td>Time division</td>
<td>( 1.0 \times 10^5 )sec</td>
</tr>
<tr>
<td>Fuel</td>
<td>n-Octane</td>
</tr>
<tr>
<td>Mobility</td>
<td>Positive ion:1, Electron:1000 cm²/Vs</td>
</tr>
<tr>
<td>Appl. voltage</td>
<td>2.4, 6 kV</td>
</tr>
<tr>
<td>Electr. Dist.</td>
<td>5cm</td>
</tr>
<tr>
<td>Init. condition</td>
<td></td>
</tr>
<tr>
<td>Gas</td>
<td></td>
</tr>
<tr>
<td>Mass frac.</td>
<td>O2:0.24, N2:0.76</td>
</tr>
<tr>
<td>Vel., Temp.</td>
<td>0cm/sec, 1200K</td>
</tr>
<tr>
<td>Liquid</td>
<td></td>
</tr>
<tr>
<td>Mass frac.</td>
<td>C8H18: 1.0</td>
</tr>
<tr>
<td>Vel., Temp.</td>
<td>0cm/sec, 300K</td>
</tr>
<tr>
<td>Droplet Dia.</td>
<td>1cm</td>
</tr>
<tr>
<td>Gravity</td>
<td>0g/cm/sec2</td>
</tr>
</tbody>
</table>
\[ S_{\text{mom}} = \frac{\pi}{6} \sum \left[ \rho_i \left( U_i^{r+1} - U_i^{r-1} \right) - \rho_i U_i^r \left( \frac{dU_i^r}{dr} \right) \right] \]  \hspace{1cm} (22)

This source is added to the gas momentum conservation equation (3) as the body force. The effect of the Coulomb force on the soot particle is defined as following:

\[ B_s = N e E \]  \hspace{1cm} (22)

It is reported that the charge number on soot \( N \) depends on the soot particle condition. In this calculation a large soot body which diameter is from 0.1 to 1.0 \( \mu \)m is adopted and number \( N \) is 14000. The soot body is considered as the integration of unordered soot particle and the represented particle which has equivalent volume with integral of large number particles is set on the field. The equivalent volume depends on the distance from the droplet surface and that is referred soot volume fraction profiles from experimental studies.

4. Results and Discussion

The direct photographs of droplet flame under various applied voltage condition which is captured in the experiment are shown in Fig.3. It can be clearly seen that the flame shape is deformed to the electrical field direction when the voltage is applied. Additionally the decreasing rate of droplet diameter is increasing with voltage applied case than that of no voltage case as shown in later.

Temperature and velocity profile which is predicted by using numerical method is shown in Fig.4, 5. Results show the profile at representative time \((t=0.3\text{sec after ignition})\). The results show that the symmetric flame shape and velocity at no applied voltage case is deformed to the electrical field direction with 4kV voltage applied case. Asymmetric profile of flow vector may cause this deformation.

The body force which causes the asymmetric velocity profile may correspond to the Coulomb force induced by electrical field. Fig.6 show the Coulomb force profile along the X-X' axis in Fig.2. Coulomb force is defined as the products of charge density and electrical field strength, furthermore the peak position corresponds to the around of flame zone. The results indicate that the ion species profile which is relative to charge and electrical field may have effect on this body force.
Fig. 7, 8, 9 shows the charge density, electrical field strength and ion species profiles respectively. Although the Coulomb force depends on both charge density and electrical field, the profile is similar to the charge density because the electrical field strength is almost 800V/cm on the X-X’ axis except for the droplet position. The effect of difference of electrical field near the flame position on Coulomb force profile may be small because of its magnitude. Charge density is relative to the integral of all ion species mass fraction shown in Fig.9. The results show that mainly $\text{H}_3\text{O}^+$ species are consisted and the other species is less than 0.1% of $\text{H}_3\text{O}^+$. Therefore the charge density depends on the profile of $\text{H}_3\text{O}^+$ strongly. The decreasing of $\text{H}_3\text{O}^+$ in $r=-0.5$ or $+0.5$ cm means that the reaction of other ion production from $\text{H}_3\text{O}^+$ is active. Actually such the area is corresponding to the peak position of temperature and other ion species. Although the dropping of the electrical field is occurred in the flame zone, both charge and electrical field strength is positive in whole field. Therefore it makes the additional momentum to the electrical field direction locally.

The comparison between experimental and numerical results about the flame deformation and time historical of droplet diameter squared is shown in Fig.10, 11. These results show that the effect of Coulomb force is underestimated in numerical prediction. In this numerical method, the soot particle formation is not considered. It is said that the soot formation includes 4 steps, nucleation, growing of surface area, oxidation and agglomeration. Even if the simplified modeling of soot formation, it is said that the concentration of acetylene have important relation with soot formation. Without this soot formation effect, sum of soot production may be underestimated.
But the burning rate constant which is defined as the gradient of the normalized droplet diameter squared is increasing with applied voltage. This result corresponds to the experimental one. The numerical predictions may be agreed qualitatively.

Increasing of burning rate constant means the faster burning velocity with electrical field. Enhancement of vaporizing droplet may be caused by increasing of amount heat flux into the droplet surface from flame. As mentioned the flame deformation which is caused by the Coulomb force make the changing of the ambient gas temperature profile. Closer flame may give much fever in the droplet and vaporizing become faster.

5. Conclusion

N-octane fuel droplet combustion flame at the electrical field under microgravity environment is investigated. Flame deformation and decreasing of the droplet diameter is captured using experimental analysis. Temperature, velocity, electrical field and some ion species mass fraction profile are predicted using numerical analysis. The mechanism of droplet vaporizing enhancement is revealed. The transfer of momentum between charge particle and bulk fluid is predicted. It is seen that the local increasing of the momentum make a flow from anode to cathode and the enhancement of vaporizing is occurred with closed flame position. The flame deformation and the burning rate constant is underestimated in numerical simulation by comparing with experimental results. It may be consider that the ignoring of soot formation inside a flame caused this discrepancy. Because of its volume fraction, the effect of soot particle on flame deformation is considerable. The simulation of soot formation should be carried out for more accurate prediction of sooting flame under uniform electrical field.

References