

Combustion Analysis of Suspended Sodium Droplet

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Abstract—Combustion analysis of suspended sodium droplet is performed by solving numerically the Navier-Stokes equations and the energy conservation equations. The combustion model consists of the pre-ignition and post-ignition models. The reaction rate for the pre-ignition model is based on the chemical kinetics, while that for the post-ignition model is based on the mass transfer rate of oxygen. The calculated droplet temperature is shown to be in good agreement with the existing experimental data. The temperature field in and around the droplet is obtained as well as the droplet shape variation, and the present numerical model is confirmed to be effective for the combustion analysis.

Keywords—Combustion, analysis, sodium, droplet.

I. INTRODUCTION

SODIUM leakage is one of the important phenomena during the core disruptive accident of sodium cooled fast breeder reactors. Sodium is highly reactive, and the leakage or discharge into the air results in fire. The spray type discharge is serious since the spray is composed of a large number of small droplets, and the reaction area between sodium and air becomes large. The understanding of the droplet combustion is thus essential for safety evaluation of fast reactors.

Experiments have been performed for the combustion of a falling sodium droplet [1], [2]. Burning rates and velocities of the droplet were measured. The combustion of a suspended sodium droplet has been observed experimentally [3], [4], and the temperature variation in the burning droplet was shown. Numerical simulations have also been performed for the falling droplet [5] and for the spray fire [6]. The droplet was, however, treated as a solid sphere in these simulations, and the characteristics of the droplet were not considered.

In this study, the analytical model for combustion of sodium droplet is proposed, and the suspended sodium droplet [4] is numerically analyzed. The analytical model consists of two stage models: the pre-ignition model and the post-ignition model. The increase in droplet temperature is compared with the existing experimental data and the flow field in and around the droplet is discussed.

II. ANALYTICAL MODEL

A. Combustion Model

The surface oxidation reaction occurs as the pre-ignition stage when the sodium droplet with relatively low temperature is released into the atmospheric air. The droplet temperature increases due to the reaction heat on the droplet surface until it reaches the ignition condition. After ignition, the combustion in

vapor phase occurs due to the evaporation of sodium from the droplet surface since the droplet temperature is sufficiently high. This is the post-ignition stage.

Two chemical reactions occur mainly during the sodium combustion.



The sodium monoxide in (1) is the main product when the droplet temperature is below 800 K [7]. It is reported for the temperature above 850 K that the reaction is composed of 60% of sodium monoxide reaction given by (1) and 40% of sodium peroxide reaction given by (2). Thus, in this study, (1) is considered for the pre-ignition stage below the droplet temperature of 850 K, and (1) and (2) are considered for the post-ignition stage above 850 K.

The surface reaction rate under relatively low temperature conditions before ignition is modeled using the chemical kinetics model [7].

$$r = \nu W_{Na} (\rho_g Y_{O_2} / W_{O_2})^n B_s \exp[-E/(RT)] \quad (3)$$

where r is the reaction rate, ν is the stoichiometric coefficient, ρ is the density, W is the molecular weight, Y is the mole fraction, n is the reaction order, B_s is the frequency factor of the surface reaction, E is the activation energy, R is the universal gas constant, T is the temperature, and the subscripts Na , g and O denote sodium, ambient gas and oxygen, respectively. The frequency factor is 320 m/s and the constant E/R is 6350 K according to the experiment [7].

The vapor phase combustion after ignition is modeled using the mass transfer rate of oxygen. The vapor reaction rate under high temperature conditions is given by [6]

$$r = 4M_o \quad (4)$$

where M_o indicates the mass transfer rate of oxygen from the ambient gas to the reaction zone. This equation corresponds to the reaction (1), and the reaction rate of sodium is four times larger than the reaction rate of oxygen. Equation (1) is considered alone in [6], and the coefficient in (4) is always four. In this study, however, the reactions (1) and (2) are considered for the post-ignition stage, and the coefficient is 4 for (1) and 2 for (2). The mass transfer rate is calculated using the mole fraction of oxygen.

$$M_o = K_c (\rho_g / W_{O_2}) (Y_{O_2} - Y_{O_2f}) \quad (5)$$

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where K_c is the mass transfer coefficient, and Y_{Of} is the mole fraction of oxygen at the reaction zone, which is calculated by taking into account the saturation vapor pressure of sodium. The mass transfer coefficient is evaluated using the following equation based on the flow field.

$$K_c = (D/d)(2.0 + 0.6Re^{0.5} Sc^{0.33}) \quad (6)$$

where D is the molecular diffusivity and d is the droplet diameter, Re and Sc are, respectively, the Reynolds number and the Schmidt number defined by the following equations.

$$Re = (\rho_g u d / \mu_g) \quad (7)$$

$$Sc = [\mu_g / (\rho_g D)] \quad (8)$$

where μ_g is the viscosity of the ambient gas.

B. Flow Field Calculation

The flow field including the burning droplet is simulated using the computational fluid dynamics (CFD) software ANSYS Fluent [8]. The Navier-Stokes equations together with the energy conservation equations are solved by the finite volume method in Fluent. The volume of fluid model is used to simulate the behavior of sodium droplet. The second order implicit method is used for time integration, and the third order monotone upstream-centered scheme for conservation laws (MUSCL) is used for spatial discretization. The pressure-implicit with splitting of operators (PISO) method is used for calculations of pressure and velocity.

The above described combustion model is implemented into the code using the user defined function of Fluent as a source term in the energy conservation equations. The energy source term is calculated by using the reaction rate.

$$S = q r \Delta s \quad (9)$$

where S is the source term in the energy equations, q is the reaction heat, and Δs is the reaction area in the calculation cell. The reaction area in the calculation cell is obtained as a function of volume fraction.

$$\Delta s = \pi l^2 \alpha (1 - \alpha) \quad (10)$$

where l is the cell size and α is the volume fraction of gas or the void fraction [9], [10]. The reaction area is zero in the pure droplet region with the gas volume fraction of zero and in the pure gas region with the gas volume fraction of unity. The cell size in (10) is given by

$$V = (\pi / 6) l^3 \quad (11)$$

where V is the volume of the calculation cell. The evaluation method for the two-phase interfacial area using (10) and (11) is very effective especially in the framework of CFD code, since

the interfacial area is not used in the governing equations for fluid motions.

The interface of two-phase flow is generally not clear in CFD codes, especially in the volume of fluid model. The volume fraction of gas is unity in the pure gas phase and zero in the pure liquid phase. The volume fraction is, however, gradually varied across the two-phase interface over several calculation cells. The interface thus has a thickness in the numerical simulation, and fluid properties such as the viscosity and the density in the interfacial region are interpolated according to the smoothly varying volume fraction. The location with the volume fraction of 0.5 is usually regarded as the interface location. The pre-ignition combustion region on the droplet surface is defined as the region with the gas volume fraction from 0.2 to 0.5, while the vapor phase combustion region is defined from 0.5 to 0.8 in this study.

C. Simulation Conditions

A single sodium droplet suspended in flowing air is simulated in the following. The simulation conditions are almost the same as those used in the experiment [4]. As shown in Fig. 1, the sodium droplet is suspended at the lower end of the vertically-oriented thin tube through which liquid sodium is pushed out. The direction of flowing air is upward. The droplet diameter is 4.0 mm and the initial temperature is 673 K (400 °C). The temperature and velocity of flowing air are 303 K (30 °C) and 0.4 m/s, respectively.

The simulation region and the initial temperature are shown in Fig. 1. The simulation region is a two-dimensional square region with a size of 12 mm x 12 mm. The simulation cell size is 0.2 mm x 0.2 mm and the number of mesh cells is thus 60 x 60. The vertical tube for suspension of droplet is also modeled. The high temperature region in the droplet is shown by red color and the low temperature region in the ambient air is by blue. The temperature in the interfacial region is gradually varied from red to blue. Square grids shown in Fig. 1 indicate the mesh cells for numerical calculations.

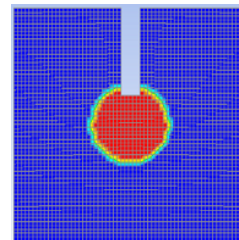


Fig. 1 Initial temperature and calculation cells

III. RESULTS AND DISCUSSION

The time history of the droplet temperature is shown in Fig. 2, along with the experimental data. It is shown that the droplet temperature increases from the initial temperature due to the pre-ignition surface reaction. The increase rate is relatively small in both the simulation and the experiment up to 0.5 s. The increase rate becomes large after 0.5 s, and the droplet temperature reaches 850 K at about 0.75 s. The temperature

shows exponential increase up to 850 K in both the experiment and the simulation. The reaction rate in the pre-ignition stage is given as the exponential function of the droplet temperature as in (3). It is found that the experimental result is represented well by the present model.

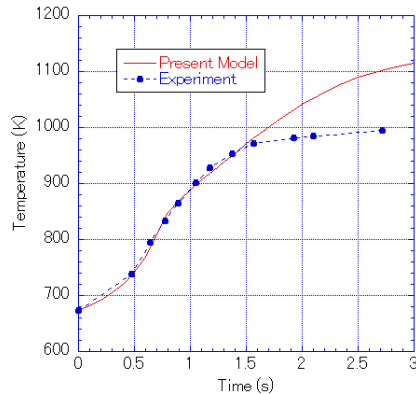


Fig. 2 Increase in droplet temperature

The increase rate of droplet temperature becomes small after ignition in both the experiment and analysis. The agreement between the experiment and analysis is good up to 1.5 s as seen in Fig. 2. The experimental droplet temperature after 1.5 s, however, reaches its maximum value of about 1000 K, while the calculated temperature continues to increase though the increase rate becomes small. The calculated temperature also seems to reach the maximum value, which is higher than the experimental data. Since the boiling temperature of sodium is about 1155 K. It is reported in the experiment that there might have been some reasons for relatively low maximum temperature in the observation [4]: the heat loss through the support tube for the droplet and the thermocouple. The heat conduction or heat capacity of the support tube is not modeled in this study, and the thermocouple is not included. The evaluation of these structural effects on the maximum droplet temperature would be desirable in the future.

The flow fields in and around the droplet such as the temperature and density distributions are shown in Figs. 3 and 4 at 1.0 s and 1.5 s, respectively. The maximum temperature in Fig. 3 is about 900 K as seen in Fig. 2, while that in Fig. 4 is about 970 K. It is shown that the high temperature region spreads widely in Figs. 3 and 4 from the droplet surface, which is indicated as the interface between the high and low density regions. Large temperature distribution is found around the droplet, especially downstream, since the ambient air flows from the bottom to the top of the simulation region.

Swinging motions and deformation are found in density distribution shown in Figs. 3 and 4. The high temperature region seems to correspond to the droplet motion, and the high temperature region is also swinging. The pre-ignition reaction occurs on the surface of the droplet, and the post-ignition reaction occurs in the vapor phase near the surface. The reaction heat, which is given by (9)-(11) as the source term in the energy equation, is added to the surface region according to

the volume fraction, and the location of source term is thus swinging corresponding to the surface motion shown in Figs. 3 and 4. The sodium droplet is treated as the solid sphere in the previous numerical simulations in the literature [2], [5], and the swinging motion and deformation cannot be reproduced. The flow field in and around the droplet including the deformation of the droplet surface is simulated in this study, and it is found that the present model with the CFD approach is very much effective to obtain the characteristics of droplet.

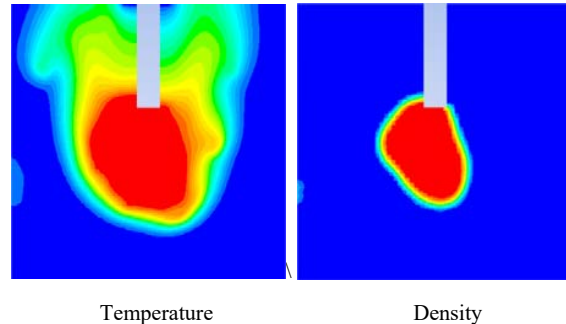


Fig. 3 Burning droplet at 1.0 s.

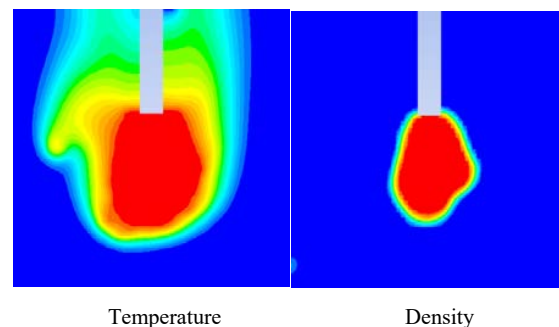


Fig. 4 Burning droplet at 1.5 s

The distributions of gas volume fraction and temperature at 1.5 s are shown in Fig. 5. The horizontal axis indicates the vertical location from the bottom in the horizontal center of the simulation region. The initial droplet center is at the location of 6 mm, which is the center of the simulation region of 12 mm x 12 mm as shown in Fig. 1. The lowest location of the vertical tube above the droplet is 7.6 mm, and thus calculated data are up to this location as shown in Fig. 5. The volume fraction indicated by red color in Fig. 5 corresponds to the left axis, while the temperature indicated by blue color to the right axis. The temperature is normalized from the minimum of 300 K to the maximum of 973 K at 1.5 s. Each symbol corresponds to the location of calculation cell. It is seen that the gas volume fraction is unity in the air and zero in the droplet. In the interfacial region at about the location of 3 mm, the gas volume fraction gradually varies from unity to zero over several calculation cells. This interfacial region corresponds to the density region in between red and blue in Fig. 4. The reaction heat is added to this region, actually to one cell with the volume fraction between 0.5 and 0.8. The temperature in the droplet is, thus, slightly lower at the location far from the interface, though

the temperature in the droplet is almost uniform.

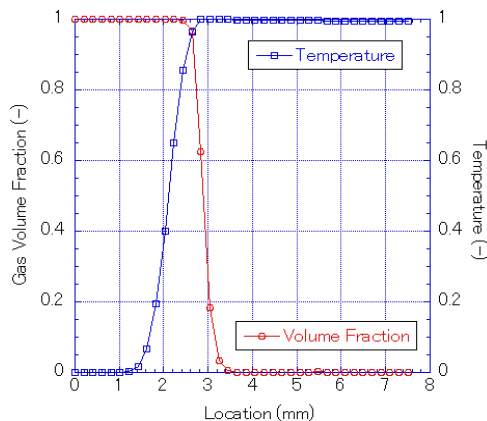


Fig. 5 Gas volume fraction and temperature

The interface region is located at about 3 mm in Fig. 5. The initial droplet center is 6 mm, and the initial diameter is 4 mm, and thus, the initial location of interface is at the location of 4 mm. It is found that the droplet deforms much in the vertical direction due to the gravity. The motion of interface or the deformation of droplet could not be simulated in the previous simulations [2], [5]. The ambient temperature increases from the location of about 1.5 mm, much lower than the droplet interface. Although the direction of ambient air flow is upward, the high temperature region is found to spread widely upstream in the gas phase. These distributions of temperature and volume fraction correspond respectively to the temperature and density shown in Fig. 4.

IV. CONCLUSION

Combustion analysis of suspended sodium droplet has been performed in this study. The flow fields in and around the droplet were obtained by solving the Navier-Stokes equations and the energy conservation equations in the framework of CFD code. The combustion model consisted of two models: the pre-ignition model and the post-ignition model. The reaction rate for the pre-ignition model was using a chemical kinetics based model, while that for the post-ignition model was based on the mass transfer rate of oxygen. The reaction heat was implemented into the code using the user defined function as the source term in the energy conservation equations.

The time variation of burning droplet was shown, and compared with the existing experimental data. The increase in temperature was shown to agree quantitatively well with the experimental data for the pre-ignition stage. Qualitative agreement was also obtained between the calculated and the experimental results for the post-ignition stage, while the maximum temperature was lower for the experiment. The swinging motion and the deformation of droplet were shown, which were not obtained in the previous numerical simulations in the literature. The spread of high temperature region into the ambient air was also shown.

The present analytical model for combustion of sodium

droplet is based on the framework of CFD code and the volume of fluid model. The volume of fluid model is widely used not only in the commercial codes but also in the open source code such as OpenFOAM, and it is easy to implement the present model into other CFD codes. The volume of fluid model is applicable for much complicated two-phase flows such as a spray including many droplets. The present model would thus be effective for detailed numerical analyses and simulations of various combustion phenomena.

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