Computational Simulation Study on the Influence of Spray/Wall Impact on the Mixing Characteristics of Bipropellant Centrifugal Apogee Engine

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Abstract. The present research investigates the impingement between spray droplets and two different coating walls is investigated to analyze effects of impingement on the mixing characteristics of propellants. In a mechanism experiment, a droplet with variable Weber number impinging on the coating walls at different wall temperatures is observed to have different behaviors, including spread, breakup, splash, suspension and rebound. Through this experiment, we establish a mathematical impinging model of these two coatings, which are identified by wall temperature and incident Weber number. These models are taken into the simulation to describe the mixing characteristics of two propellants under thermal atmosphere. The results indicate a significant difference in the mixing situation for two coatings impingement, showing a good agreement with experimental results of firing tests. Compared with SiCrTiZr coating, MoSi2 coating significantly benefits better mixing to improve combustion efficiency with lower temperature simultaneously, because more droplets get into impingement regimes of rebound and participate into central combustion. Therefore, oxygen-rich combustion area is centralized away from chamber wall, which is conducive to survival of liquid cooling film.

Keywords: Bipropellant engine; Coating wall; Spray droplets; Model; Simulation.

1. Introduction
Since the Apollo Space Program, bipropellant liquid engine has been playing an essential role in the attitude and orbit control of spacecrafts. Centrifugal engine has been widely used in many propulsion systems as a mainstream solution. It is well known that fuel MMH and oxidizer NTO sprayed from a swirl injector into the chamber participate in the combustion to power the spacecraft after fine atomization, fast evaporation and effective mixing. However, as for a centrifugal apogee engine, atomization quality of swirl injector is limited because of low supply pressure provided in the propulsion system with higher flow rate. Thus, it requires a long process to achieve full atomization and evaporation. And those unevaporated droplets impinge on chamber wall and generate a series of behaviors, such as sticking, spread, splash and rebound. Some of droplets stick to the wall and form a cooling film, and others splash or bounce back into chamber for further mixing and combustion. Therefore, the research on spray/wall impact directly affects engine’s combustion and working temperature, which has a considerable significance of engine performance.

In the ESA/ESTEC Technology Research Program, the ROCFLAM (Rocket Combustion Flow Analysis Module) [1] was developed to run simulations for liquid-film cooled bipropellant rocket engines. It is focused on the formation of cooling film on the platinum alloy smooth wall, which
interacts with propellant droplets and gas flow on the boundary layer. It was validated by calculations with different injection characteristics for 400N engine. However, as for a coating wall with rough morphology, the situation could be more different and complicated, because the interaction between droplets and coating wall has totally different mechanisms.

In the research of droplet impingement, Naber and Reitz [2] proposed the famous N-R model in 1988 to judge the impinging behaviors based on Weber number. They divided the droplet/Wall impinging behaviors into three states: adhesion, rebound and injection. Bai and Gosman [3] [4] considered the influence of wall temperature and defined a detailed impingement model based on both Weber number and wall temperature. Lee and Ryu [5] then developed an impingement mechanism judged by Weber number and wall temperature into nine categories. Naber and Farrell et al. [6] employed the experiment of an impingement between a single droplet and hot wall. They divided the thermodynamic states into four types: liquid-film evaporation state, boiling state, transition state and Leidenfrost state. Pierre Dunand [7] researched the problem of droplets impinging the wall, when wall temperature was higher than Leidenfrost point. In his work, the two-color method was used to measure splash droplets’ temperature and obtain detailed characteristic parameters. Mitrakusuma [8] [9] conducted an experiment to investigate effects of wettability on impingement between a droplet with medium impact Weber number and a hot wall. Al-Roub and Farrell [10] studied the process of droplet impingement on the wall with liquid film. Their researches indicated that liquid film has a significant effect on the spray impinging behavior. Stanton [11] analysed the mechanism of spray-film interaction in detail and established a two-dimensional model of liquid film evolution.

In the field of droplet’s impingement on a rough wall, Rioboo et al. [12] and Moita et al. [13] summarized influence of various factors on the impinging mechanism. They gave following qualitative conclusions. Roughness of smooth wall \( (R_a/R_0<3.4e^{-4}) \) led to unstable liquid film, while roughness of rough wall \( (R_a/R_0>2.5e^{-3}) \) cause collapse of film, where \( R_a \) was the average wall roughness and \( R_0 \) was droplet initial radius. When wall roughness increased, it promoted rapid splashing and finger-like fragmentation, but inhibited corona splash and partial rebound. Randy et al. [14] and M. Bussmann [15] carried out researches about the effect of wall roughness on the droplet impinging characteristics. They analysed the correlation between dimensionless surface average roughness \( (R_a/D_0) \) and splash parameter \( K_c \), where \( D_0 \) was droplet diameter.

With the aid of computational technology development, numerical simulation has gradually become an effective solution to research droplet impingement. Mahulkar et al. [16] [17] researched the process of impingement under the condition of a hot wall employing LES (Large Eddy Simulation). Chia-Fon Lee et al. [18] conducted simulations of spray impingement under the presence of liquid film by DPM (Discrete Phase Model) method and obtained vapor concentration distribution near the wall. Nikolopoulos et al. [19] carried out a two-phase continuous flow simulation. They used VOF (Volume of Fluid) method to analyse splash characteristics of an impingement between droplets and filmed wall. In terms of spray/wall interaction research, Andreassi et al. [20] used experimental methods to analyse the characteristics of spray/wall impact, and then ran the simulation with Bai-Gosman model. This study verified the applicability of that model for a cold wall. Frank Robert Held et al. [21] also studied the spray impingement on a high-temperature wall by means of simulative comparison.

To sum up, there are many factors influencing on the spray/wall impingement. For many bipropellant engines, the chamber wall must be coated with high-temperature resistant oxidation coating. So impinging situation in the firing process is very complicated because of high-temperature and rough wall. And it is difficult to model coating wall surface with complex morphology. In this paper, based on experimental results and classical models of other researchers, new mathematical models adapted to this problem is established. These impinging models are used to evaluate subsequent evaporation and mixing under high temperature and rough wall boundary conditions.

2. Mechanism Experiment

2.1. Experimental System Introduction

The mechanism experiment is focused on the development of a single droplet when it impinges on a coating wall under given temperature conditions. In this experiment, kinematic characteristics of liquid
droplet need to be investigated for mathematical model construction. A high-speed camera with microscopy was used to capture more details of impingement between a single droplet and a coating wall. A droplet generator can produce a droplet with 1.5mm diameters. The temperature control system was consisted of an electric heating plate, a thermocouple and a thermal controller. They constructed a controlled heat condition on a coating wall. A long micro lens was used to distinguish kinematic characteristics of droplet when it impinged on the wall. The experimental system of droplet/wall impingement is shown in Figure 1.

Figure 1. Experimental system of droplet/wall impingement with high-speed camera and microscope

Weber number is a dimensionless ratio of inertial force and surface tension [22]. When Weber number is much larger than 1, the effect of surface tension is relatively small, so the difference of liquid property on droplet/wall impingement is also slight. Due to the strong corrosive and toxic characteristics of propellants, water was used to replace MMH and NTO. The generated particle size of a droplet is 1.5mm, so its incident Weber number only depends on incident velocity of the droplet. This velocity is determined by controlling height of droplet generator, which makes incidence Weber number range from 0 to 2500 and cover injection condition in the chamber, including a variety of droplets from small and low-speed to large and high-speed.

In order to improve authenticity of this experiment, two kinds of real coating samples were used, as shown in Figure 2. Sample 1 was a SiCrTiZr coating with a rough surface and irregular morphology. It was prepared by slurping method. Its surface roughness was about 4.5 microns. Sample 2 was a MoSi2 coating made by vacuum ion plating and infiltration method. Its surface was relatively smooth with some local silicide bumps and roughness of around 2 microns.

Figure 2. Two coating wall samples used in droplet impingement experiment

In the experiment, the incident Weber number of a droplet was gradually increased from small to large for observation. Since the boiling point $T_B$ of water at standard pressure is 100°C, and the Leidenfrost temperature $T_L$ defined as the temperature at which the droplet rebounds from the insulating vapor layer is around 190°C. Therefore, the range from room temperature to 250°C can cover several mechanisms of impingement when the droplet impacts on the coating wall. At room temperature, there is no heat transfer with wall surface, so the mechanism is relatively simple. When the incident Weber number of a droplet is greater than 596, the surface of sample 1 starts to form a coronal splash. However, for sample 2, only when the incident Weber number increases up to 852, the splash phenomenon occurs. It indicates that the coating surface morphology does have a significant effect on
the behavior of droplets after impact.

![Image of droplet impingement at different wall temperatures](image)

**Figure 3.** A droplet’s impingement on sample 1 at different wall temperature

| Wall temperature: | 100°C | 150°C | 200°C | 250°C |
|-------------------|-------|-------|-------|-------|

When wall temperature $T_w$ is lower than $T_b$, the droplet spreads and then forms a liquid film after impingement, which is like the situation of impinging on a cold wall. With the increase in $T_w$, it changes from spread to splash or rebound mechanism. Because liquid film is strongly disturbed under the boiling condition, coupled with the decrease of liquid surface tension at higher temperature. In this way, the spread film is more likely to break up with a finger-like structure. Meanwhile, as $T_w$ goes up, the splashing speed is also accelerated. When wall temperature $T_w$ exceeds $T_l$, many suspended and broken droplets appear obviously on the surface of sample 1, as shown in Figure 3. And after
impinging on sample 2, droplets mainly break up and bounce back, as shown in Figure 4.

Figure 4. Effect of two different coatings on the broken droplet’s behavior

Compared with sample 2, sample 1 has a more considerable surface roughness and a looser surface structure. It is easy to form many micro-holes at the solid-liquid interface. It leads to an increase in apparent thermal resistance and a decrease in heat flux between solid and liquid. By contrast, Sample 2 has a low surface roughness and smooth surface morphology. It reduces the probability of cavitation formation, and its apparent thermal resistance is smaller than that of sample 1. When a droplet comes to the Leidenfrost state, the lower apparent thermal resistance improves the evaporation rate of the wall-attached liquid, causing the broken droplet to get more prominent propulsion force and rebound speed to move away.

2.3. Impingement Regimes and Transition Conditions

After getting all information, like speed, size and number of droplets after impingement in the experiment, we constructed the classification of impingement regimes and transition conditions, as shown in Figure 6. The vertical coordinate is the incident Weber number of droplets, and the horizontal coordinate is wall temperature.

Figure 5. Effect of two different coatings on the broken droplet’s behavior

Compared with sample 2, sample 1 has a more considerable surface roughness and a looser surface structure. It is easy to form many micro-holes at the solid-liquid interface. It leads to an increase in apparent thermal resistance and a decrease in heat flux between solid and liquid. By contrast, Sample 2 has a low surface roughness and smooth surface morphology. It reduces the probability of cavitation formation, and its apparent thermal resistance is smaller than that of sample 1. When a droplet comes to the Leidenfrost state, the lower apparent thermal resistance improves the evaporation rate of the wall-attached liquid, causing the broken droplet to get more prominent propulsion force and rebound speed to move away.

Figure 6. Comparison of impingement regimes and transition conditions

The main difference between these two different coatings can be explained in two aspects. Firstly, the critical Weber number of regimes transition condition is different. The critical weber number of the relatively smooth wall is higher than that of the rough wall. When wall temperature is below the Leidenfrost point, the rough wall only needs the critical Weber number of 596 to generate a splash, while the smooth wall requires 862 Weber number. Secondly, when the temperature of the wall surface is higher than Leidenfrost point, the critical Weber numbers of SiCrTiZr coating and MoSi2 coating are 426 and 639, respectively.
3. Numerical Simulation

3.1. Model Construction

Many impingement models of other researchers are combined with experimental results. Bases on that, an impingement model of coating wall can be constructed for correction and fitting. Figure 7 shows normal velocity \(v_b\), tangential velocity \(u_b\), droplet size \(d_b\) and splash angle \(\theta_b\) of droplet before impingement, as well as normal velocity \(v_a\), tangential velocity \(u_a\), droplet size \(d_a\) and splash angle \(\theta_a\) of droplet after impingement. According to the difference of \(T_w\), the discussion can be divided into three cases: (1) \(T_w < T_B\), (2) \(T_B \leq T_w < T_L\), and (3) \(T_w \geq T_L\). The model of SiMo$_2$ coating was introduced in detail in our work with Pengfei Fu [23] [24], as shown in Table 1.

![Figure 7. Illustration of a droplet’s impact on the wall](image-url)

**Table 1. The mathematical model of liquid droplet’s impact on the wall with MoSi$_2$ coating**

| Criterion | Splash velocity | Splash Angle | The mass of splash droplets | The diameter of splash droplets |
|-----------|-----------------|--------------|----------------------------|-------------------------------|
| When wall temperature is lower than the droplet boiling point, that is, \(T_w < T_B\) | \(v_0 = -83.75e^{-0.086\cdot T_w} + 1.44\) | \(\theta_0 = 0.623 \cdot \theta_b + 2\) | \(d_{1}\) \(=\) 0.5 \(\cdot d_b\) (parcels 1); \(d_{2}\) \(=\) 0.9 \(\cdot d_b\) (parcels 2); Distribution of the droplet’s diameter: \(f(d) = \frac{5}{8} (\frac{d}{d_0})^3 e^{-\left(\frac{d}{d_0}\right)^2}\) | \(N_1 = 5 \cdot \left(\frac{W_{ena}}{W_{enb}} - 1\right)\) (parcels 1); \(N_2 = Na - N_1\) (parcels 2). |
| When wall temperature is between the droplet boiling point and the Leidenfrost temperature, that is, \(T_B < T_w < T_L\) | \(v_0 = 3.435\cdot T_w^{-0.117}\) \(\cdot u_b\) is same as above. | Idem. | Idem. | Idem. |
| When wall temperature is above the Leidenfrost temperature, that is, \(T_w > T_L\) | When \(W_{ena} \leq 106\), \(v_a = 0\) | \(\theta_a = 0.623 \cdot \theta_b\); When \(W_{ena} > 106\), \(W_{ena} = 2719\cdot W_{enb}^{-1.28}\), \(u_a = u_b\); When \(W_{ena} > 639\), \(v_0 = 0.0582 + (-4.514/(58.98 - \sqrt{W_{ena}}))\cdot e^{(-3.58\cdot W_{ena}/(9.98\cdot W_{ena}))}\). | When \(W_{ena} \leq 639\), \(d_{ena} = d_{enb}\); When \(W_{ena} > 639\), it is the same as above. | \(d_{ena} = 1.375e^{0.011W_{ena}}\). |

In the model of MoSi$_2$ coating, prediction of mass ratio and quantity of splash droplets are based on the description of Bai-Gosman model. Distribution model of Stanton and Rutland [25] is employed to
describe characteristics of splash droplets size. By using the model of Kalantari and Tropea [26], splash parameters can be defined as well. The mathematical relationship established in those classical models was still followed in the model construction. However, coefficients in this model must be fitted according to experimental results, such as diameter and velocity of splash droplet. By contrast, the model of SiCrTiZr coating is similar to that of MoSi2 coating, when $T_w$ is lower than $T_l$. The only difference is the different critical Weber number in classification. When $T_w$ is higher than $T_l$, the model of SiCrTiZr coating changes greatly, and leads to significant effect on mixing and combustion. When $W_e < 426$ at high $T_w$, we can get $v_a = 0$, $u_a = u_b$ and $d_a = d_b$ because of the suspension of droplet. When $W_e \geq 426$, droplet splashes and suspends. The velocity of splashed droplet is fitted in accordance with experimental data and expressed as,

$$v_a / u_b = 7 \times 10^{-5} \cdot W_e^{1.362}. \quad (1)$$

In terms of splashed droplet’s size, when $W_e < 800$, it is determined by the incident Weber number and expressed as,

$$d_a / d_b = -2 \times 10^{-5} \cdot W_e + 0.563. \quad (2)$$

When $W_e \geq 800$, the velocity of splash droplet decreases dramatically with the increase in the incident Weber number, according to the experimental data. Thus, it can be described as,

$$d_a / d_b = 57114 \cdot W_e^{1.72}. \quad (3)$$

In this case, normal velocity of suspended droplet is 0, and tangential velocity remains equivalent to that of incident droplet. Figure 8 shows the fitting results of velocity and diameter of splash droplet.

![Figure 8. The relationship between We and splash velocity (left) and splash diameter (right)](image)

3.2. Simulation Results

The governing equation of engine combustion process was solved by RANS method. And the chemical reaction of NTO/MMH was evolved under the condition of thermal atmosphere. Propellant droplets injected into the combustion chamber were simulated via DDM (Discrete Droplet Model) method. The injection process from a swirl nozzle can be described by using LISA Model (Linearized Instability Sheet Atomization Model), which is based on the theoretical analysis of liquid film instability [27] [28]. The EBU (Eddy Breakup Model) was used as the turbulent model in KIVA3V, with the new impingement model obtained from the experiment. The initial pressure and temperature in the simulative domain were 0.95MPa and 3000K, respectively.

After droplets of MMH and NTO are injected into the combustion chamber, they subsequently impinge on chamber wall without enough time for evaporation. Under the heating effect of wall surface, vapor of MMH and NTO began to form after spray/wall impingement. Because of the different interaction with different coating walls, distribution of MMH vapor and NTO vapor can change greatly, as shown from Figure 9 to Figure 12.
Figure 9. Contour image of MMH vapor distribution with SiCrTiZr coating wall

Figure 10. Contour image of NTO vapor distribution with SiCrTiZr coating wall

For an engine with SiCrTiZr coating, more droplets of NTO tend to suspend near the chamber wall and then evaporate there after impingement. Figure 9 and Figure 10 indicate that the concentration distribution of NTO vapor and MMH vapor get separated, leading to a poor mixing with a negative effect on combustion efficiency and film cooling. As for diffusion combustion, the poor mixing requires more time and space for completed chemical reactions. Especially for the coating wall with a temperature limit, it is risky that a high oxygen-rich area is formed near the chamber wall. Because it can form extremely high-temperature burning gas due to its high equivalence ratio. This situation further increases wall temperature and worsens the survival condition of liquid film attached to the wall. That may shorten the service life of bipropellant apogee engine.

In Figure 11 and Figure 12, we can figure out the notable difference in the concentration distribution of NTO vapor and MMH vapor. The mixing of oxygen-fuel vapor is more uniform and centralized, and the mixing area overlapped by two propellants increases obviously. That is conducive to the formation of central high-temperature flame and the improvement of combustion efficiency. When wall temperature is low, because the critical Weber number of MoSi2 coating is much higher than SiCrTiZr coating, liquid film can spread more in the low-temperature region to cool the engine’s injector. When wall temperature is higher than boiling point, induced breakup of liquid film begins. When it comes to the Leidenfrost state, droplets are likely to rebound to central region, subsequently evaporate and further participate in combustion.
3.3. **Comparison with the Firing Test Results**

In a sea-level firing test, two engines with different coatings were tested for a comparison. Experimental data showed that, compared with MoSi2 coating, not only the specific impulse of engine coated with SiCrTiZr was decreased by 3s, but also the surface temperature of combustion chamber measured by the infrared thermal imager was much higher, as shown in Figure 13.

![Contour image of MMH vapor distribution with MoSi2 coating wall](image1)

**Figure 11.** Contour image of MMH vapor distribution with MoSi2 coating wall

![Contour image of NTO vapor distribution with MoSi2 coating wall](image2)

**Figure 12.** Contour image of NTO vapor distribution with MoSi2 coating wall

According to test data of infrared thermography, maximum temperature of engine with SiCrTiZr coating was 317°C higher. And the high-temperature area was obviously larger and close to the upstream injector. The high-temperature situation is very risky for engine’s service life. Meanwhile, its
lower performance reflects that nonuniform vapor distribution and poor mixing significantly worsen combustion efficiency.

4. Conclusion
By conducting an experiment of droplet impingement on two different coating walls, a mathematical model is constructed with different classifications of impingement regimes and transition conditions. Through the simulation of propellant mixing based on new model and infrared data in the firing test, it shows that the effect of coating wall surface morphology on combustion efficiency and film cooling is significant for bipropellant centrifugal apogee engine.

(1) Surface morphology of different coatings significantly affects classifications of impingement regimes and transition conditions. Firstly, the rough wall surface is more likely to make droplet splash. Secondly, the rough wall morphology tends to make droplets suspend under the condition of high incident Weber number and high-temperature wall, while the smooth wall surface is more likely to get the droplet rebound.

(2) At high temperature, the effect of wall roughness on droplet spread is weakened by the presence of vapor layer between droplet and wall surface. The rough coating wall can strengthen heat transfer at solid-liquid interface, and enhance the evaporation of droplets.

(3) The propellant mixing in the engine chamber is different in two cases of different coating walls. SiCrTiZr coating tends to cause the problem of oxygen-rich high temperature near the wall with a negative effect on combustion and cooling. For the engine with MoSi2 coating, more uniform mixing can be formed to improve the combustion efficiency and cooling performance.

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