Numerical Investigation of the Thermal Behavior of Cracked RP-3 in Rectangular Cooling Channels under Different Inclinations

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ABSTRACT: The pyrolysis effect of aviation kerosene is common in the regenerative cooling process of hypersonic aircraft scramjets. To find out the effect of inclination variation on the characteristics of aviation kerosene RP-3 considering thermal cracking in a regenerative cooling rectangular channel, a detailed chemical mechanism of RP-3 pyrolysis is introduced to construct a numerical model. The results indicate that the pyrolytic reaction begins at the junction of the heating wall and the side walls, and the main products of pyrolysis are light olefins and alkanes. The thermal cracking reaction slows down the velocity of the main flow on account of the increased density and increased viscosity resulting from the decrease in RP-3 temperature. With the decrease in inclination, thermal cracking is enhanced and the average heat transfer coefficient is decreased, which leads to an increase in wall temperature.

INTRODUCTION

For the thermal protection of scramjets, regenerative cooling has been widely associated with advantages in weight and cost compared to passive thermal protection, film cooling, and their combinations. The principle of regenerative cooling is to cool down the inner wall of the combustion chamber with flowing aviation kerosene, which participates in combustion afterward. Aviation kerosene normally works at a supercritical state, where the physical parameters dramatically vary with the pressure and temperature of the flow field. During the process of regenerative cooling, when the kerosene temperature exceeds a threshold level, complex thermal cracking occurs, obviously impacting the fuel heat transfer and combustion efficiency.

Numerous experimental and computational studies have been carried out to explore the thermal performance of aviation kerosene in the regenerative cooling process, wherein a large proportion of the numerical focused on the influence of the geometric size, the buoyancy effect, or the coupled effect of several factors on the heat and mass transfer of supercritical kerosene. For instance, Zhu et al. numerically investigated the effect of the vertical tube diameter on heat transfer deterioration of buoyancy under supercritical pressure; the results argued that heat transfer deterioration was aggravated with a smaller diameter such as when the diameter of the tube was below 10 mm. Wang et al. focused on the non-uniform heat transfer deterioration of RP-3 and found that the abnormal stratification caused by buoyancy triggered non-uniform heat transfer deterioration, which can be weakened by decreasing the outer-wall heat flux, increasing the pressure, and increasing the mass flux. The results obtained by Sun et al. indicate that low inlet flow velocities, high electric currents, and large diameters contribute to a significant influence of buoyancy on heat transfer. Most experiments about RP-3 are conducted to obtain physical properties, flow patterns, and thermoacoustic oscillation. Deng et al. measured isobaric heat capacity data of RP-3 temperatures in the range of 292.1−823.9 K and pressures in the range of 2.40−5.98 MPa, and the critical and pseudo critical temperatures at different pressures were obtained. On account of the complexity of pyrolysis, the research mentioned above was conducted without consideration of the thermal cracking process, and this led to the deviation between the numerical results and practical situation.

In recent years, the pyrolysis effect of aviation kerosene has been closely followed. However, most investigations laid stress on the heat and mass transfer of kerosene in horizontal tubes, vertical tubes, or serpentine tubes, which is rarely concerned with the most common rectangular channel. To the best of our knowledge, the inclination of the rectangular
channel has also received little attention, and the effect of inclination on kerosene thermal behavior has not been figured out.

In the article, a detailed model is introduced to investigate the influence of inclination on pyrolysis, flow, and heat transfer inside the rectangular cooling channel. The model was based on the surrogate fuel proposed by Yu et al. The conversion of RP-3 in the pyrolytic process is compared under different inclinations. The temperature of the bulk fluid and wall as well as the flow field inside the regenerative cooling passage are also analyzed to reveal the effect of thermal cracking and variation of inclinations.

### SIMULATION MODELS AND BOUNDARY CONDITIONS

The schematic of the regenerative cooling passage is presented in Figure 1. The size of the entire rectangular channel is 2 × 2 × 600 mm, and the channel is only heated on one side at the bottom, z = 0 mm. The length of the heating section in the channel is 300 mm, as shown in the red part of Figure 1a. An adiabatic inlet section of 150 mm is provided to ensure that the turbulent flow is fully developed. At the same time, a 150 mm adiabatic outlet section was set up to reduce the influence of outlet boundary conditions and the back flow of the aviation kerosene flow in the channel. As shown in Figure 1c, the angle between the gravity direction and the flow direction is set as θ + 90°, and θ is the inclination angle of the rectangular channel.

The mass flow rate of the inlet is $q_{in} = 3$ g/s ($v_{in} = 1.05$ m/s), and the temperature of the inlet is $T_{in} = 373$ K. The boundary of the outlet is set as the pressure outlet of $p = 5$ Mpa. According to the experimental results from Zhang et al., the peak heat flux of combustor sidewalls can be more than 2000 kW/m². Therefore, $q = 1500$ kW/m² and $q = 2000$ kW/m² are chosen as two typical heat fluxes.

In this research, the variation of the inclination angle $\theta$ is from 0 to 90°. When $\theta = 0°$, supercritical RP-3 flows horizontally in the channel; when the inclination angle is positive, the kerosene flows upward in the channel.

### SIMULATION METHOD

The governing equations are expressed as follows:

Momentum conservation

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0$$

Energy conservation

$$\frac{\partial}{\partial x_i}(\rho u_i u_j - u_i \tau_{ij} + q_j - S_j) = 0$$

Species conservation

$$\frac{\partial}{\partial x_i}(\rho u_i y_k) = \frac{\partial}{\partial x_i}\left(\frac{\partial y_k}{\partial x_i}\right) + \alpha_k$$

Compared with other turbulence models, the RNG $k-\varepsilon$ model has a higher calculation accuracy in high-speed flow, vortex flow, and complex flow with variable physical properties. To better simulate the turbulent flow process and heat transfer inside the regenerative cooling channel with pyrolytic reaction, the RNG $k-\varepsilon$ model was introduced in the work. To improve the computational accuracy, the enhancement wall treatment is applied. The turbulent kinetic energy and turbulent kinetic dissipation equation are expressed below

$$\frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_i}\left(\alpha_h \frac{\partial k}{\partial x_i}\right) + G_k + G_b - \rho \varepsilon - Y_m + S_k$$

$$\frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_i}\left(\alpha_h \frac{\partial \varepsilon}{\partial x_i}\right) + C_{1e} \frac{\varepsilon}{k} (G_k + C_{2e} G_b) - C_{2e} \rho \varepsilon^2 - R_e - S_\varepsilon$$

where the values of $C_{1e}$, $C_{2e}$, and $C_{3e}$ are 1.42, 1.68, and 0.0845, respectively.

### CHEMICAL KINETIC MODEL

Considering that aviation kerosene has a great variation in compositions and involves hundreds of chemical components with different molecular structures, constructing a model considering all components of aviation kerosene is rather difficult and onerous. Thus, a simplified surrogate fuel model consisting of several component species is regarded as an effective solution. In the study, a three-component surrogate fuel model proposed by Yu is adopted. The chemical reaction mechanism containing 28 components and 79 elementary reactions is obtained by simplifying the reaction mechanism of the three-component substitution model of RP-3 aviation kerosene.

The expression of the kinetic model is

$$\sum_{i=1}^{N} \alpha A_s \rightarrow \sum_{i=1}^{N} \beta A_s$$

The mass formation rate per unit volume of the component is obtained by the laminar finite rate model as follows

$$S_i = 0.001 M_i (\beta_i - \alpha_i) R_i$$

$$R_i = k_A \prod_{j=1}^{N} \left( q_j / 0.001 M_j \right)^{\alpha_j}$$

$\sum_{i=1}^{N} \alpha A_s \rightarrow \sum_{i=1}^{N} \beta A_s$
The reaction rate constant \( k_A \) is calculated by the Arrhenius expression.

\[
k_A = AT^\theta e^{-E_a/RT}
\]

### VALUATIONS

The numerical results simulated by four sets of mesh with quantities of 1,632,960, 2,062,500, 2,625,000, and 3,240,000 are compared to verify grid independence. It should be emphasized that the mesh in the boundary layer is refined to obtain higher accuracy. By contrast, the grid with 2,625,000 meshes renders less than 0.1% relative numerical error in terms of average temperature in the channel. Thus, the set of grids of 2,662,500 is chosen to complete the subsequent computation. So far, the research on supercritical aviation fuel is basically carried out in the horizontal circular tube, which is supported by many experimental and simulation data, and the numerical method used in this paper also has a certain generality in the research of flow heat transfer in the circular tube. Therefore, the convective heat transfer of supercritical RP-3 aviation kerosene in the horizontal tube was simulated by the numerical method used in this paper, and the simulation results were compared with the experimental results obtained by Zhang et al.\(^\text{30}\) and the numerical simulation results from Ren et al.\(^\text{31}\) (Figure 2)

![Figure 2. Comparison of the wall temperatures.](image)

### RESULTS AND DISCUSSION

When \( q = 2000 \text{ kW/m}^2 \) and \( \theta = 0^\circ \), the temperature, velocity, and mass fraction of RP-3 along the mainstream and on the outlet are presented in Figure 3. To qualitatively understand the influence of thermal cracking on heat transfer and flow, the temperature distribution, velocity variation, and mass fraction of RP-3 along several lines in the \( y-z \) section are also computed in Figure 3. The wall temperature of the heating section is nearly 1000 K, which is far more than the pyrolysis temperature of 800 K, and it makes thermal cracking initiate from the heating wall. The wall temperature drops drastically at the end of the heating section, which results from the absence of the external energy input and the lasting pyrolysis effect. When \( z = 0.4 \text{ mm} \), the temperature decrease at the end of the heating section is evident since the impact of wall temperature drop is not dismissed and leads to the heat being transferred from RP-3 in the middle part of the passage to the fluid near the heating wall. From the figure, the temperature decreases first and then increases slightly from \( y = 0.45 \text{ m} \) to \( y = 0.6 \text{ m} \), which is explained by the secondary reaction between pyrolytic products and the end of the reaction.

![Figure 3. Temperature (a), velocity (b), and mass fraction of the RP-3 (c) distribution in the flow direction (x = 0 mm) and the outlet section of the heating section (y = 0.45 m) after coupling cracking reaction.](image)

From the velocity distribution illustrated in Figure 3b, with the increase in the aviation kerosene temperature, the flow core area gradually approaches the heating surface, and the maximum flow rate is significantly improved. The flow velocity variation at the beginning of the heating section is distinct. When \( z = 0.4 \text{ mm} \), the pyrolysis production accelerates the
flow and makes the flow velocity increase when RP-3 enters the heating section.

The mass fraction of RP-3 is negatively correlated with the conversion, so the degree of thermal cracking can be inferred from the mass fraction distribution. As shown in Figure 3c, when RP-3 flows to the heating section, the decreasing mass fraction of RP-3 near the heating surface indicates the occurrence of thermal cracking. Figure 4 shows the RP-3 mass fraction of the x−z section at several crucial positions during the development of thermal cracking. The thermal cracking reaction starts at $y = 0.17$ m, and it is noted that $Y_{RP-3}$ at the position where the heating surface and the side wall intersect is first below 1. The position has the highest degree of cracking reaction due to the low velocity and the highest temperature of kerosene. Along the main flow direction, the cracking reaction first diffuses to the entire heating wall, as shown by $y = 0.18$ m. With the development of the flow, the pyrolytic products diffuse to the region far from the heating wall, where the temperature is below the threshold temperature but the mass fraction decreases. When $y = 0.29$ m, all kerosene is cracked into low-carbon hydrocarbons. In the whole heating section, the position with the highest degree of cracking occurs at $y = 0.4$ m, and the maximum cracking rate reaches 38%.

Figure 5 shows the distribution of several major cracking products along the main flow direction when $q = 2000$ kW/m$^2$ and $\theta = 0^\circ$. The product mass fraction in Figure 5a is significantly larger than that in Figure 5b, indicating that under the condition of $q = 2000$ kW/m$^2$, the main cracking products of aviation kerosene are these light hydrocarbons and olefins. In Figure 5a, the trend of mass fractions of the two alkanes is changed. When the maximum cracking rate of aviation kerosene reaches 25%, the mass fractions of these two alkanes begin to increase, which inhibits the increase in the aviation kerosene cracking rate. It can be regarded as the main product of the secondary reaction.

Figure 6 shows the comparison of the fluid temperature of RP-3 along the mainstream direction with and without cracking reaction when $\theta = 0^\circ$. The temperature of the bulk fluid gradually increases along the flow direction under continuous heating. Due to endothermic cracking reaction, the bulk temperature is lower when pyrolysis is considered. Moreover, compared with the situation of $q = 1500$ kW/m$^2$, the pyrolysis effect on temperature decrease is more obvious, and the temperature difference appears earlier when $q = 2000$ kW/m$^2$. It can be attributed to the enhancement in thermal cracking of RP-3 at a high heating flux.

Figure 7 compares the distribution of the mainstream velocity of RP-3 aviation kerosene along the mainstream direction with and without cracking reaction when $\theta = 0^\circ$. With the progress of the cracking reaction, the main flow velocity decreases, but the variation in the main flow velocity is

![Figure 4. Mass fraction of RP-3 distribution along the main flow direction.](image1)

![Figure 5. Distribution of main cracking products (a) and minor cracking products (b) at $q = 2000$ kW/m$^2$ and $\theta = 0^\circ$.](image2)

![Figure 6. Comparison of temperature distribution along the main flow direction at $\theta = 0^\circ$.](image3)

![Figure 7. Comparison of velocity distribution along the main flow direction with and without cracking reaction when $\theta = 0^\circ$.](image4)
small under the condition of $q = 1500 \text{ kW/m}^2$ with a lower cracking degree. The cracked products are all low-carbon hydrocarbons, and their density and viscosity are much smaller than those of supercritical RP-3 aviation kerosene, which leads to an increase in the fluid velocity. However, the cracking reaction also causes a decrease in the mainstream temperature, which is responsible for an increase in the density and viscosity of aviation kerosene with the largest mass fraction in the channel and a decrease in the mainstream velocity. Considering the changes in the physical properties of supercritical RP-3 aviation kerosene and the effects of cracking products, the increase in the cracking rate reduces the mainstream velocity of aviation kerosene. At the same time, the decrease in the mainstream speed will prolong the residence time of RP-3 aviation kerosene in the channel and further improve the cracking rate of aviation kerosene.

**DISCUSSION ON THE EFFECT OF INCLINATION**

As illustrated in Figure 8, the inclination variation of the rectangular channel plays a significant role in the degree of pyrolysis. The average conversion of RP-3 shows an increasing trend with the decrease in the tilt angle. The trend is pronounced at $q = 1500 \text{ kW/m}^2$, and the average conversion when $\theta = 0^\circ$ is nearly 0. According to the analysis from Yu et al., the increase in the inclination angle will not only weaken the secondary flow intensity in the channel but also cause the wall temperature to decrease significantly. Thermal cracking is an endothermic reaction affected by wall temperature a lot; thus the decrease in wall temperature leads to a decrease in conversion. Meanwhile, the weakening of the secondary flow makes it rather difficult to exchange energy. Therefore, at a lower heat flux density, the increase in the inclination angle will significantly reduce the cracking rate.

When the heat flux density is $q = 2000 \text{ kW/m}^2$, the average cracking rate of the section is larger, and the influence of the inclination angle on the cracking rate is small. The change in the maximum cracking rate in the $x-z$ section is analyzed. Figure 9 shows the distribution of the maximum cracking rate along the main flow direction at different inclination angles. It can be seen from the figure that along the mainstream direction, the maximum cracking rate keeps increasing, but when it reaches 25%, there is a slow decline process, and then, the maximum cracking rate continues to increase and can reach up to 38%. When $\theta = 0^\circ$, the cracking rate is the largest, and from $\theta = 45^\circ$ to $\theta = 90^\circ$, the maximum cracking rate of the two is close and does not increase with the increase in the inclination angle. The trend of the product mass fraction in Figure 5a is consistent with the trend of the maximum cracking rate of aviation kerosene, which also verifies that these light hydrocarbons are the main products of primary cracking reaction.

Figure 10 shows the trend of the wall temperature of the heating surface along the main flow direction with and without the cracking reaction at different inclinations of $q = 1500 \text{ kW/m}^2$. The wall temperature decreases when inclination increases with or without crack. The basic reason for variation is the heat transfer enhancement with the increase in the inclination angle. The chemical heat sink provided by the cracking reaction can effectively reduce the wall temperature. The higher the cracking rate, the greater the drop in wall temperature. As analyzed before, the pyrolysis effect makes a contribution to
inhibit the main flow of RP-3, and the absence of the pyrolysis effect strengthens the flow. With the decrease in inclination, the pyrolysis effect is exacerbated and the wall temperature is lowered. In the working condition of $\theta = 90^\circ$, where the cracking rate is extremely low, the wall temperature still drops significantly, which has a good alleviation effect on the harsh working environment of the regenerative cooling channel. However, it can also be seen that along the mainstream direction, the wall temperature fluctuates significantly, and the secondary reaction has a greater impact on the local wall temperature. Figure 11 shows the variation of the average secondary flow velocity along the main flow direction of the cross-section with coefficient of other inclination angles, indicating that with the development of the cracking reaction, it strengthens the heat transfer coefficient. The influence of the inclination angle has been exceeded.

**CONCLUSIONS**

In the article, a detailed chemical model is applied to model the thermal cracking process of aviation kerosene RP-3 in a rectangular regenerative cooling channel, and the variation of channel inclination on the thermal behavior of RP-3 and the regenerative cooling effect is discussed. The following conclusions are obtained.

1. The pyrolysis reaction starts at the junction between the heating and side walls. The increase in the cracking rate helps to reduce the temperature of aviation kerosene. The increase in RP-3 conversion leads to a decrease in the main flow velocity in the channel, which increases the residence time of RP-3 aviation kerosene in the cooling channel, further strengthening the degree of cracking reaction. The main products of the primary cracking reaction are light olefins and alkanes, and the secondary reaction inhibits the primary cracking reaction of RP-3 aviation kerosene.

2. As the inclination of the regenerative cooling channel decreases, the average conversion of the RP-3 increases significantly. However, the average heat transfer coefficient decreases and the wall temperature increases, which is harmful to the regenerative cooling efficiency. The secondary velocity increases as inclination increases.

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Notes
The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

This study is funded by the Open Fund of Chongqing Key Laboratory of Fire and Explosion Safety (no. LQ21KFJJ02), the Open Fund of State Key Laboratory of High-Temperature Gas Dynamics (no. 2021KF14), and Natural Science Foundation Project of Chongqing, Chongqing Science and Technology Commission (no.cstc2021jcyj-msxmX0658).

■ NOMENCLATURE

Latin Letters
A pre-exponential factors, s⁻¹
C_p constant-pressure specific heat, J/(mol·K)
D_s diffusion coefficient of species s, m²/s
E_a activation energy, J/mol
h_s enthalpy of species s, kJ/kg
k thermal conductivity, W/(m·K)
\(k_A\) Arrhenius rate constant, 1/s
P pressure, MPa
q heat flux, W/m²
\(q_m\) mass flow rate, kg/s
R universal constant, 8.314 J/(mol·K)
S source term
T temperature, K
u velocity, m/s
x axial coordinate, m
y axial coordinate, m
Y mass fraction
\(z\) axial coordinate, m
\(Z\) concentration of aviation kerosene
\(\rho\) density of aviation kerosene, kg/m³
\(\theta\) inclination of the channel
\(\lambda_t\) turbulent thermal conductivity, W/(m·K)

Subscripts
in inlet of the channel
out outlet of the channel
w wall

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