INVESTIGATION ON MICRO-FLAME STRUCTURE OF AP COMPOSITE PROPELLANT UNDER WIDE PRESSURE RANGE

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Abstract: This present work proposes a method to exactly evaluate the thermal process of Ammonium perchlorate/Hydroxyl-terminated polybutadiene (AP/HTPB) propellant. The three-dimensional propellant pack is generated by the Monte-Carlo method to obtain a representative sandwich model on the base of the dual-slicing technique. The AP monopropellant flame height $H_1$, the primary diffusion flame height $H_2$ and the final diffusion flame height $H_3$ are jointly determined by the temperature and component distributions of the gas phase thermodynamic field, which is more accurate to capture this complicated combustion field distribution of the gas phase comparing with earlier reported studies. Peclet number and Damkohler number are also introduced to quantitatively investigate the influence mechanism of chemical kinetics and diffusion mixing process of components on this micro-flame structure under wide pressure range (0.69MPa-20.7MPa). Further, based on the criterion of whether the premixed flow above the burning surface can absorb heat flux continuously from the diffusion flame to approach adiabatic flame temperature, the diffusion flame is divided into two regions in detail: (1) flame front and (2) trailing diffusion flame.

Keywords: AP/HTPB propellant; BDP model; diffusion flame; thermal process.

1. Introduction:

Ammonium perchlorate/Hydroxyl-terminated polybutadiene (AP/HTPB) propellant is widely used in the fields of ground launch systems with drag-reduction equipment, solid rocket motors for missiles and rocket launchers due to its high specific impulse, good ignition characteristics, and predictability of the burning rate. However, the combustion process of this composite propellant is very complicated based on the fact that a dispersion of discrete random AP particles in a fuel binder matrix, involving thermal decompositions of multiple solid compositions, gas-solid coupling, premixing and diffusion reactions of gaseous reactants. Further, the premixing and diffusion reactions of combustion gases are particularly affected by the combustion pressure, AP particle size, and binder content. To explore the complex reaction process of the gas zone, Beckstead et al proposed the BDP model, dividing the AP/HTPB combustion process into three coupled flame structures: AP monopropellant flame, primary diffusion flame, and final diffusion flame. Price et al observed the micro-combustion characteristic of composite solid propellant under lower combustion pressure by high-speed photography, which verified the accuracy of the BDP model. Gross et al developed the BDP model and used a series of modified parameters from
the micro-scale model to establish a global dynamic meso-scale combustion model, in which a four-step reaction mechanism was used to describe the gas-flame structure of AP/HTPB propellant.

To describe the reaction of the gas phase more specifically in the combustion process of the AP/HTPB propellant, Buckmaster et al. [2] introduced the Peclet number \((Pe)\) and Damkohler number \((Da)\) to define the relative size of convective-to-diffusive transport rates as well as the chemical reaction and diffusive transport rates. The values of \(Pe\) and \(Da\) are closely related to the temperature, species, gas phase heat release rate, burning rate, and other physical quantities. Chorpening et al. [5] further investigated the combustion characteristics of AP/HTPB propellant by adjusting the \(Pe\) and \(Da\), which obtained the following conclusions: (1) The \(Pe\) is related to the burning rate and the binder thickness; (2) \(Da\) is related to the pressure and the binder thickness; (3) Low \(Pe\) and low \(Da\) make the products of AP and HTPB more fully mixed. There is a strong correlation between \(Pe, Da,\) and the volume heat release.

To explore the premix and diffusion degree of gaseous reactants in the combustion process of AP/HTPB propellant, the concept of flame height is proposed. It is a comprehensive function of the pressure, AP particle size, and binder content. Beckstead et al. [2] pointed out that the AP monopropellant flame and the primary flame are competing for the oxidizing gas in the wide range of pressure. Moreover, since AP/HTPB propellant is heterogeneous in nature with a multi-modal distribution of AP particles embedded in the HTPB polymer matrix, the overall gas flame of AP/HTPB propellant is composed of multiple micro-structure flames. This micro-distribution of heterogeneous AP/HTPB propellant that affected this micro-flame structure can be described by the symmetrical arrangement structure of two AP particles and mutually enwrapped HTPB, which is called the sandwich model. It was first proposed by Powling [6]. The most prominent advantage of the sandwich model is that the flame structure can be observed systematically, which is also the reason why there are so many theoretical studies on the sandwich model [7-10]. Knott et al. [11] employed this sandwich model and then selected the Oseen approximation method to eliminate the momentum equation along the \(x\) direction, coupling the gas-solid reaction to study the influence of the environment pressure on the flame structure. Chorpening et al. [5] conducted extensive experiments of observing flame structure by ultraviolet emission and transmission imaging two-dimensional configuration of laminae of AP and HTPB, which also verified the numerical results of Knott et al. [11].

The importance of solid-phase modeling, especially the reaction of condensed phase, heat transfer, and the distribution of AP particle size has been acknowledged by early models. The approximations with different degrees were also used to simulate real AP/HTPB propellant and then improve computational accuracy and efficiency. Jackson et al. [12] first proposed a simplified model that can simulate the internal structure of the composite propellant. Knott et al. [13] developed a random particle packing algorithm, which treated AP crystals as disks(2D) or spheres(3D). The model was very helpful to simulate the combustion of AP/HTPB propellant, which can be used to obtain the influence of the distribution of AP particles on the burning rate characteristics of this composite propellant. Massa et al. [14] examined the combustion process of AP/HTPB propellant by using a simplified three-step
reaction mechanism based on this random particle packing algorithm. Vijay et al\textsuperscript{[15]} used X-ray computed tomography (XCT) technology to reconstruct the real three-dimensional AP/HTPB propellant packing and compared it with the random particle packing in the AP exposed area and AP/binder intercept lengths, which confirmed the accuracy of the proposed model used for numerical simulation. However, the solution of the random distribution model needs to consume numerous computational resources. To accurately investigate the burning behaviors of AP/HTPB from the micro level and simplify the calculation requirements, Vijay et al\textsuperscript{[16]} sliced the generated random particle packing to obtain the representative sandwich model and then used it to calculate the burning rate of AP/HTPB propellant. Compared with the experimental data of Miller\textsuperscript{[17]}, Ishitha and Ramakrishna\textsuperscript{[18]}, and Kubota and Miyazaki\textsuperscript{[19]}, the results showed that the model was successful in predicting the burning rate of AP/HTPB propellant.

In this work, the focus is to develop a method to exactly evaluate the micro-AP/HTPB combustion that is generated by the Monte-Carlo method and then intercepted by dual-slicing technology introduced according to Vijay’s report\textsuperscript{[16]}. Subsequently, the gas-solid coupling model and the BDP model of AP/HTPB propellant with micro-scale are established and are used to study the micro-components reaction mechanism and heat flow exchange characteristic of this AP/HTPB propellant in a larger range of environment pressure from 0.69MPa to 20.7MPa in more detail by numerical simulation. A comprehensive evaluation method using $Pe$, $Da$, and flame heights is proposed quantitatively to explain the chemical kinetics and diffusion mixing process of the gas-phase combustion region of AP/HTPB propellant. Further, the diffusion flame is divided into flame front and trailing diffusion flame based on the criterion of whether the premixed flow above the burning surface can absorb heat flux continuously from the diffusion flame to approach adiabatic flame temperature.

2. Numerical model

2.1 Generation and intercept method of AP/HTPB propellant with a random particle packing

The bridge to represent real AP/HTPB solid propellant by using a representative sandwich is the establishment of the three-dimensional random model, where the most important process is the selection of AP particle size and number. Since different AP particle sizes are embedded into the HTPB binder, the burning rate and micro-flame structure of AP/HTPB propellant will be significantly affected. Miller\textsuperscript{[17]} used 400μm, 200μm, 20μm, 5μm or even smaller AP particles to synthesize 29 non-aluminized propellants to obtain experimental burning rate data base, providing the data available for comparison with various theoretical models\textsuperscript{[26,33,34]}. In this paper, based on Miller’s experiment\textsuperscript{[17]}, three types of AP/HTPB propellant structures (SD III-16, SD III-22, and SD III-24) with an AP particle loading rate of 86% are established by the Monte-Carlo method. The proportions of different sizes of AP particles and HTPB layer are shown in Table 1, and the structure is shown in Fig.1, where pink spheres represent 400μm AP particles, red spheres represent 200μm AP particles, blue spheres represent 50μm AP particles, and yellow spheres represent 20μm AP particles.
### Table 1. The Proportion of different particles in AP/HTPB propellant\(^{[17]}\)

<table>
<thead>
<tr>
<th>Composition</th>
<th>Mass fraction of AP (%)</th>
<th>400μm</th>
<th>200μm</th>
<th>50μm</th>
<th>20μm</th>
<th>14</th>
</tr>
</thead>
<tbody>
<tr>
<td>SD III-16</td>
<td>0</td>
<td>31</td>
<td>31</td>
<td>24</td>
<td></td>
<td>14</td>
</tr>
<tr>
<td>SD III-22</td>
<td>31</td>
<td>0</td>
<td>41</td>
<td>14</td>
<td></td>
<td>14</td>
</tr>
<tr>
<td>SD III-24</td>
<td>0</td>
<td>31</td>
<td>41</td>
<td>14</td>
<td></td>
<td>14</td>
</tr>
</tbody>
</table>

**Fig. 1.** Structure diagram of three types of AP/HTPB propellant

Using the technique of Vijay et al.\(^{[16]}\), three kinds of AP/HTPB structures are firstly performed by multiple surface cuttings, as shown in Fig.2, and then 50 planar slices with an interval of 15μm are generated. Fig.2(b) shows the distribution of AP and HTPB on one of the slices (the circle represents AP particles, and the area not occupied by the AP particles in the slice is the binder in the propellant). Subsequently, 25 linear cuttings with an interval of 30μm are performed on the generated multi-group slices, that is, a group of parallel lines are used to continuously cut the section. The half intercepts made by the AP particles on the lines are taken as AP particle sizes and the half regions on the line which are not intercepted by AP particles are taken to be the HTPB thickness. Finally, the sizes of AP and HTPB obtained by multiple linear cuttings are averaged, and the relationship between them is obtained, as shown in Fig.2 (c) and (d). It can be seen from Fig.2 that the HTPB thicknesses of SD III-16, SD III-22, and SD III-24 propellant packages remain stable at 7μm, 6μm, and 5μm after 400 times cutting. After cutting 3500 times, the AP sizes remain steady at 21μm, 14μm, and 12μm.

**Fig.2.** Diagram of cutting method. (a) three-dimensional AP/HTPB propellant structure; (b) AP/HTPB planar slice; (c) variation curve of AP intercept with cutting times; (d) variation curve of HTPB intercept with cutting times

However, Vijay et al.\(^{[16]}\) did not present whether the AP and HTPB intercepts of the sandwich model are necessarily related to the length of the three-dimensional box. Since the ‘representative’ sandwich model is the micro-structure of the three-dimensional AP/HTPB propellant, they should have similar combustion characteristics, that is, a ‘representative’ sandwich model represents a kind of AP/HTPB propellant. it is necessary to verify the size independence. Taking SD III-22 propellant as an example, three kinds of propellants with lengths of 800 μm, 900 μm, and 1000 μm are produced and cut according to the above
method. The results are shown in Fig. 3. It can be seen from the Figure that under the premise of the same AP loading rate and the same proportion of different particle sizes, the intercepts of AP and HTPB keep stable with the change of the three-dimensional AP / HTPB propellant size. Based on this principle, the ‘representative’ sandwich models of AP / HTPB propellants with three different structures are established respectively.

2.2 Physical model

According to the AP and HTPB intercepts in Table 2, the representative sandwich models of SD III-16, SD III-22, and SD III-24 AP/HTPB propellants are established, as shown in Fig. 4. The oxidant AP is located in $L_1 < |x| < L_2$ and the binder HTPB lies in $|x| < L_f$. To simplify the calculation, the following assumptions are proposed.

1. Boggs and Hightower et al. [20-21] found bubbles and ridges exist above the quenched surface of AP, which proved that there was a melting layer near the burning surface, and thus most of the heat flux in the gas phase is transferred to the solid phase by thermal conductivity. To simplify the calculation, thermal feedback only considers the thermal conductivity of the gas relative to the burning surface.

2. The oxidant AP and binder HTPB are regarded as two independent components with different thermophysical parameters, the solid phase pyrolysis reaction occurs on the burning surface layer, and only the heat conduction effect is considered in the solid phase.

3. Assuming that the gas is the ideal gas and the Lewis number of all components of the gas phase is 1. Moreover, the gas thermal conductivity $\lambda_g$ is the function of temperature.

4. The thermal decomposition of solid propellant is described by zero-order Arrhenius law, and the gas phase combustion process of AP/HTPB is described by the BDP flame model combined with the two-step global reaction mechanism.

5. The pressure is uniformly distributed throughout the gas phase on a micro-scale.

2.3 Mathematical model

2.3.1 Chemical kinetic equation

The combustion of AP/HTPB is divided into two processes including the solid phase and the gas phase. The physical and chemical phenomena of the solid phase process include AP and HTPB preheated by heat conduction and endothermic pyrolysis of these two components, and thus the corresponding solid region is also divided into the solid preheating zone and solid reaction zone. The solid phase reaction zone is located on the solid phase surface, which is the
melting layer. The AP component undergoes the following thermal decomposition reactions:

\[
\text{AP}(s) \xrightarrow{\Delta Q_{\text{c,AP}}} \text{NH}_3(g) + \text{HClO}_4(g) \quad (1)
\]

HTPB undergoes the following pyrolysis reaction:

\[
\text{HTPB}(s) \xrightarrow{\Delta Q_{\text{c,B}}} \frac{C_2H_4(g)}{2} \quad (2)
\]

where the formula of (1) is an exothermic reaction, the decomposition heat is expressed as \(Q_{\text{c,AP}}\); equation (2) is an endothermic reaction, the decomposition heat is expressed as \(Q_{\text{c,B}}\).

Zero-order Arrhenius law was used to describe the pyrolysis rates of two solid components:

\[
\dot{m}_{\text{AP}} = \rho_{\text{AP}} A_{\text{AP}} \exp(-E_{\text{AP}}/R_u T_{\text{AP,S}}) \quad (3)
\]

\[
\dot{m}_{\text{B}} = \rho_{\text{B}} A_{\text{B}} \exp(-E_{\text{B}}/R_u T_{\text{B,S}}) \quad (4)
\]

where \(\rho_{\text{AP}}\) and \(\rho_{\text{B}}\) represent the density of oxidant AP and binder HTPB, \(A_{\text{AP}}\) and \(A_{\text{B}}\) are pyrolysis rate constants, \(E_{\text{AP}}\) and \(E_{\text{B}}\) are pyrolysis activation energy of oxidant AP and binder HTPB, respectively; \(T_{\text{AP,S}}\) and \(T_{\text{B,S}}\) are the burning surface temperature of oxidant AP and binder HTPB, \(R_u\) is the general gas constant.

The pyrolysis products of the solid phase are used as the reactant of the gas phase process, and the two-step global reaction mechanism based on BDP multi-flame model is used to describe the combustion process of the gas phase reaction:

\[
\frac{\text{NH}_3(g) + \text{HClO}_4(g)}{2} \xrightarrow{\Delta Q_{\text{c,final}}} \text{O}_2(g) + \text{H}_2\text{O}(g) + \text{HCl}(g) + \text{N}_2(g) \quad (5)
\]

\[
\frac{C_2H_4(g)}{2} \xrightarrow{\Delta Q_{\text{c,final}}} \text{CO}_2(g) + \text{H}_2\text{O}(g) + \text{HCl}(g) + \text{N}_2(g) \quad (6)
\]

where component \(\tilde{X}\) represents \(\text{NH}_3(g) + \text{HClO}_4(g)\), component \(\tilde{Y}\) on behalf of \(C_2H_4\), component \(\tilde{Z}\) is \(\text{H}_2\text{O}(g) + \text{HCl}(g) + \text{O}_2(g) + \text{N}_2(g)\). respectively, \(\beta\) represents the AP mass required to consume 1kg HTPB, and the Arrhenius law is employed to describe chemical reaction rates \(R_1\) and \(R_2\).

\[
R_1 = D_1 P^{n_1}[X] \exp\left(-\frac{E_1}{R_u T}\right) \quad (7)
\]

\[
R_2 = D_2 P^{n_2}[Y] [Z] \exp\left(-\frac{E_2}{R_u T}\right) \quad (8)
\]

where \(D_1\) and \(D_2\) are pre-exponential factors, \(n_1\) and \(n_2\) represent pressure indexes; \(E_1\) and \(E_2\) are the reaction activation energy, respectively, \([X], [Y], [Z]\) are the mass fractions of components \(\tilde{X}, \tilde{Y},\) and \(\tilde{Z}\), subscripts 1 and 2 correspond to the first step and the second step reaction.

2.3.2 Solid-phase equation

The solid phase only considers the thermal conduction process and is expressed as:

\[
\rho_c c_c \frac{\partial T}{\partial t} = \frac{\partial}{\partial y} \left( \lambda_c \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial x} \left( \lambda_c \frac{\partial T}{\partial x} \right) + s_c \quad (9)
\]

Where \(\rho_c\), \(c_c\), \(\lambda_c\) and \(s_c\) are density, specific heat, thermal conductivity, and energy source term of solid phase, respectively.

\[
\lambda_c = \begin{cases} \lambda_B, & \rho_c = \rho_B, \quad c_c = c_B, \quad |x| < L_1 \\ \lambda_{\text{AP}}, & \rho_c = \rho_{\text{AP}}, \quad |x| < L_2 \end{cases}
\]
2.3.3 Gas-phase equation

The multi-component Navier-stokes equation in the plane rectangular coordinate system is established for the gas phase.

Continuity equation:

\[ \frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \vec{V}) = S_m \]  

Momentum equation:

\[ \frac{\partial (\rho_g \vec{V})}{\partial t} + \nabla \cdot (\rho_g \vec{V} \vec{V}) = -\nabla p + \frac{1}{3} \nabla (\mu_g \nabla \cdot \vec{V}) + \Delta (\mu_g \vec{V}) + S_{mom} \]  

Components equation:

\[ \rho_g (u \frac{\partial Y_i}{\partial x} + v \frac{\partial Y_i}{\partial y}) = \nabla \cdot (\rho_g D_{ij} \nabla Y_j) + S_i \]  

Energy equation:

\[ \rho_g C_p \left( u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \nabla \cdot (\lambda_g \nabla T) + S_{eng} \]  

State equation:

\[ \rho_g R_u T = p M_u \]  

where \( \rho_g \), \( \mu_g \), \( c_p \), \( \lambda_g \), and \( M_u \) are the density, viscosity coefficient, constant pressure specific heat capacity, thermal conductivity, and molecular molar weight of the gas. \( D_{ij} \) is the binary diffusion coefficient of one of the components in the mixture. \( R_u \) is the general gas constant. \( Y_i \) is the mass fraction of the components. \( \vec{V} = (\vec{u}, \vec{v}) \), and \( \vec{u} \) and \( \vec{v} \) are velocity components along the x and y directions respectively. \( S_m, S_{mom}, S_i, \) and \( S_{eng} \) are the terms of mass source, momentum source, component source, and energy source.

The thermal conductivity \( \lambda_g \) of gas is the function of temperature \( T \):

\[ \lambda_g = 1.08 \times 10^{-4} T + 0.0133 \]  

The gas viscosity \( \mu_g \) is the function of the thermal conductivity \( \lambda_g \):

\[ \mu_g = \frac{\rho r \lambda_g}{c_p} \]  

2.3.4 Equivalent source term method

Assuming that the phase transition occurs in a thin layer of the burning surface, the source terms are added into this layer of the grid to represent the mass flow of the burning surface, namely:

\[ \dot{m} = \rho_c r_b \]  

where

\[ r_b = \begin{cases} 
  r_B = A_B \exp\left(-\frac{E_B}{R_u T_s}\right) & |x| < L_1 \\
  r_{AP} = A_{AP} \exp\left(-\frac{E_{AP}}{R_u T_s}\right) & L_1 < |x| < L_2 
\end{cases} \]  

To ensure the continuity of the burning rate at the AP/HTPB interface, the burning rate at the interface of two components of solid is modified by the method of reference \(^{[22]}\):

\[ r_B = r_B^{0.25} r_{AP}^{0.75} \]  

The corresponding gas mass source, momentum source, energy source, component \( \vec{X} \) source, component \( \vec{Y} \) source, and component \( \vec{Z} \) source terms can be expressed as:
\[
\begin{pmatrix}
S_m \\
S_{mom} \\
S_{eng} \\
S_x \\
S_y \\
S_z
\end{pmatrix} =
\begin{pmatrix}
\frac{\rho c^2 T_b}{\Delta y} \\
\rho c^2 T_b \hat{V} \\
\frac{\rho c^2 T_b \hat{V}}{\Delta y} \\
\sum Q_{g,i} R_i \\
- R_1 \\
- R_2
\end{pmatrix}
\]

(19)

where \(\Delta y\) represents the grid length of the combustion surface layer, \(R_i\) and \(Q_{g,i}\) are the reaction heat and reaction rate of step \(i\) (namely, \(R_i\) represents \(R_1\) and \(R_2\)).

The energy source terms of oxidant AP and binder HTPB can be expressed as:

\[
\begin{pmatrix}
S_{e,AP} \\
S_{e,B}
\end{pmatrix} = \begin{pmatrix}
\frac{\rho_{AP} c^2 T_{e,AP}}{\Delta y} \\
\frac{\rho_{B} c^2 T_{e,B}}{\Delta y}
\end{pmatrix}
\]

(20)

2.3.5 Gas-phase coupling relationship

In the combustion process, the gas-solid interface temperature keeps continuous, namely:

\[
T|_{y=0^+} = T|_{y=0^-}
\]

(21)

where \(0\) represents the burning surface, \(0^+\) represents the gas phase side of the burning surface, and \(0^-\) represents the solid phase side of the burning surface.

The mass flux on the burning surface remains balanced, namely:

\[
\rho_g V_g = \rho c \hat{r}_b
\]

(22)

where \(V_g\) is the gas velocity.

The components balance at the burning surface can be expressed as:

\[
\dot{m}_{Y_i}|_{y=0^+} - \rho_g D_{Y_i} \frac{\partial Y_i}{\partial y}|_{y=0^+} = \dot{m}_{Y_i}|_{y=0^-}
\]

(23)

where \(D_{Y_i}\) is the average binary diffusion coefficient of gas.

The heat flux balance at the burning surface can be expressed as:

\[
\lambda_g \frac{\partial T}{\partial y}|_{y=0^+} + \rho c \hat{r}_b Q_c = \lambda_c \frac{\partial T}{\partial y}|_{y=0^-}
\]

(24)

2.3.6 Boundary conditions and calculation methods

Because the left and right boundaries are symmetrical, only half of the region, that is, the part of model \(x > 0\mu m\), is calculated. The axial length of the solid phase is 500\(\mu m\), and the axial length of the gas phase is 700\(\mu m\). There are the following boundary conditions for the solid-phase far field, gas-phase far field, and symmetric boundary:

The far field of the solid phase:

\[
T|_{y=-\infty} = 300k
\]

(25)

The far field of the gas phase:

\[
\frac{\partial Y_i}{\partial y}|_{y=+\infty} = 0 \quad Y_i = T, \bar{X}, \bar{Y}, \bar{Z}
\]

(26)

Symmetric boundary:

\[
\frac{\partial F}{\partial x}|_{x=0, \pm L_2} = 0 \quad F = \bar{u}, \bar{v}, T, \bar{X}, \bar{Y}, \bar{Z}
\]

(27)

The boundary conditions of gas-solid interface:

\[
\begin{align*}
Y_2 &= 0, Y_{\bar{Y}} = 1, Y_{\bar{Z}} = 0 \quad \text{if} \quad |x| < L_1 \\
Y_2 &= 1, Y_{\bar{Y}} = 0, Y_{\bar{Z}} = 0 \quad \text{if} \quad L_1 < |x| < L_2
\end{align*}
\]

(28) (29)
After the grid independence test, the grid division method is determined as follows: the grid size is 0.5μm by using uniform grid division along the x direction; the gas phase and solid phase regions along the y direction adopt the tapered grid, where the minimum grid size with 0.5μm is located in both sides of the burning surface and the maximum grid size with 1.69μm is located in the far field of gas phase and solid phase. At the same time, the numerical calculation is carried out based on the finite volume method. The pressure-velocity coupling adopts the Simple scheme, and the density, mass, momentum, and component equations adopted the second-order upwind scheme. The physical parameters can be seen in Ref. [22].

3. Validation of the calculation model

As can be seen from Fig.5, the calculated average burning rates of SD III-16 and SD III-22 are in reasonable agreement with experimental results, and the average errors calculated by Eq. (30) are 2.43% and 7.01%. The calculated burning rates of SD III-24 under high-pressure conditions deviate slightly from experimental values, and the average error is 10.0%. Vijay et al. [16] and VarunKumar [23,24] pointed out that the density and temperature sensitivity of propellant also affected the burning rate, which is rarely reported in previous literature. It is a possible reason to cause a deviation between the calculation results and the experiment reported results.

\[
\text{Mean absolute percentage error} = \frac{1}{m} \sum_{i=1}^{m} \left| \frac{\text{pre}_i - A_{ci}}{A_{ci}} \right|
\]

where, \( r_b(x, y, z) \) is the local burning rate, \( \bar{r}_b \) is the average burning rate and \( A \) is the burning surface area. The \( \text{pre}_i \) represents the calculated value, \( A_{ci} \) represents the experimental value, and \( m \) represents the number of local burning rate points.

The burning rate plays an important role to characterize the performance of the rocket engine and ground launch vehicle, the relationship between the burning rate and the propellant working pressure satisfies an exponential relation of Eq. (31).

\[
\bar{r}_b = ap^n
\]

where the constant \( a \) is the burning rate at unit pressure, and the constant \( n \) is the pressure index. By fitting the average burning rate curves of AP/HTPB with different structures under different pressures in Fig.5 (d), the values of \( a \) and \( n \) in Eq. (33) are obtained as shown in Table 2, which is consistent with the AP/HTPB pressure index in the range of 0.4-0.6 given in Ref. [11].

<table>
<thead>
<tr>
<th>Case</th>
<th>Burning rate at unit pressure ((a))</th>
<th>Pressure exponent ((n))</th>
</tr>
</thead>
<tbody>
<tr>
<td>SD III-16</td>
<td>0.596</td>
<td>0.448</td>
</tr>
<tr>
<td>SD III-22</td>
<td>0.529</td>
<td>0.481</td>
</tr>
<tr>
<td>SD III-24</td>
<td>0.498</td>
<td>0.457</td>
</tr>
</tbody>
</table>
Fig. 5. The comparison of average burning rate.

4. Effect of environment pressure on the micro-combustion characteristic

4.1 Gas-phase heat release rate of the micro-combustion field.

Heat release is a proportional measurement of the reaction strength and flame structure in the gas phase. Fig. 6 shows the contours of the gas-phase heat release rate under different environmental pressures for SD III-22 AP/HTPB propellant. When the environment pressure is 0.69 MPa, the reaction rate is slow. Thus, components $\tilde{Y}$ and $\tilde{Z}$ have sufficient time to mix. Compared with high-pressure conditions, the core of the heat release rate is larger and far away from the burning surface. As the pressure increases, the core area of the gas-phase heat release rate decreases and moves towards the AP/HTPB interface. At the same time, the diffusion flame develops continuously, and two bands of independent diffusion flame are gradually formed. Chorpening et al.\cite{5} found that the micro-flames with 120μm–160μm sandwich propellants were separated through the experiments when the pressure reached to 3.2MPa. The representative sandwich model used in this paper is only 20μm, and the flame shows a stronger premixed effect. So, the flame separation occurs delayed. When the pressure rises to 13.8MPa or above, the AP monopropellant flame moves closer to the burning surface while the final diffusion flame becomes taller and more concentrated along the stoichiometric surface.

Fig. 6. Gas-phase heat release rate under different pressures for SD III-22

An increase in pressure increases the gas-phase energy production rate, this in turn influences the heat flux to the AP/HTPB propellant. The burning surface thermal feedback profiles (Fig.7) demonstrate how the overall heat flux to the solid phase become under
different pressures. It can be seen that the thermal feedback distribution of the whole burning surface is relatively balanced under low-pressure condition. With an increase of the operating pressure, the thermal feedback of the AP side is significantly higher than that of the HTPB side, which is consistent with the experimental results of Price et al [3]. At the same time, there is an increasingly peak near the AP/HTPB interface. This because only the species near the oxidizer fuel interface can fully react and produce more combustion heat. Taking the simulation of 13.8MPa as an example, the peak value of this heat feedback is 138.37W·m⁻², the thermal conductivity at the center of AP is 95.6W·m⁻², and the heat flux at the center of HTPB is 27.20W·m⁻². That is to say, the maximum heat feedback of the burning surface under this environment pressure is 1.48 times and 5.08 times than that above AP and HTPB, which is also the main reason that the local burning rate of AP is greater than that of HTPB.

Fig.7. Thermal feedback distribution under wide pressure range

The predicted temperature profiles of the micro-combustion field under different ambient pressures are shown in Fig.8. To examine various combustion characteristics of the micro-flame structure of AP/HTPB propellant, the angle β of 2420 K temperature contour above the oxidizer fuel interface is introduced to analyze temperature distribution characteristics of the gas phase. β are calculated as 107° for 3.45MPa, 63° for 6.89MPa 26° for 13.8MPa 20° for 17.25MPa and 15° for 20.7MPa, respectively. The reason for the variation of β is explained as follows.

The diffusion length scale at a certain binder width is determined by the ambient pressure. As environmental pressure increases, the species from the oxidizer and fuel mix incompletely before reacting. Therefore, a non-dense reaction zone formed in the vicinity of the HTPB surface. This results in the gas temperature gradually changing from uniform to ‘W’ type distribution, so an increase in pressure decreases the value of β. This trend gives an indirect proof reference [5,25] reported the splitting of the base of the flame structure as well as the numerical result of Fig.6.
Fig. 8. Gas-phase temperature distribution with different pressures for SD III-22

4.2 Effects of environment pressure on combustion components $\tilde{X}$ and $\tilde{Z}$

The distribution of components $\tilde{X}$ and $\tilde{Z}$ under different pressures are shown in Fig.8. It can be seen from the Fig.9 that component $\tilde{X}$ is mainly distributed above AP. Its distribution area decreases considerably with an increase in ambient pressure from 0.69MPa to 20.7MPa. When the pressure is 3.45 MPa, the height of the zone $H_\tilde{X}$ where component $\tilde{X}$ content is greater than 0.01 above the AP center is 7.2μm. When the pressure is 20.7MPa, $H_\tilde{X}$ is only 2.5μm. This is because the reduction characteristic time for species reactions makes the consumption of component $\tilde{X}$ easier in the reaction step ($R_1$), the predicted trend of component $\tilde{X}$ is consistent with the BDP model [2].

Since component $\tilde{Z}$ is both the product of AP decomposition reaction $R_1$ and the reactant of diffusion-reaction $R_2$, the influence of chemical reaction and diffusion process on micro-combustion characteristic can be further explained by analyzing the distribution characteristic of component $\tilde{Z}$. When the environment pressure is 0.69MPa, the distribution core of component $\tilde{Z}$ is slightly away from the burning surface. Its homogeneous distribution and the low content indicate that fuel vapors and oxidizer steam can fully diffuse and mix in the reaction $R_2$. With the increase in pressure, larger areas are seen to be at higher gas phase heat release, which facilitates the second step of the reaction ($R_2$). The angle $\alpha$ of the contour where the content of component $\tilde{Z}$ above AP is 0.01 along the $+x$ is 68° for 6.89MPa; as the ambient rises to 20.7MPa, $\alpha$ is 82°. The larger and larger region of activity of component $\tilde{Z}$ becomes more difficult for component $\tilde{Y}$ to diffuse into the steam above AP. At the same time, when ambient pressure is 6.89MPa or above, nearly all of component $\tilde{Z}$ concentrate on the AP side, in accordance with the predicted flame separation phenomenon given in Fig.6.
Fig. 9. Components $\tilde{X}$ and $\tilde{Z}$ distributions of SD III-22 under different pressures

4.3 Effects of environment pressure on micro-flame heights

As mentioned above, the micro-combustion flame structure of AP/HTPB propellant is very complex, so the concept of flame height is introduced to explore the influences of environmental pressure on its flame structure. Hedmon and co-workers [26,27] applied high-speed planar laser-induced fluorescence (PLIF) to measure diffusion flame formed by different types of propellant. However, there is some uncertainty (i.e., surface compositional fluctuations and irregularities in the measurement process) in measuring the flame height during the experiments; on the other hand, since the AP monopropellant flame length scales are very short, it is difficult to measure its height due to insufficient spatial resolution. Accurate numerical models are needed to capture more details on flame, which benefits the development of new measurement techniques. Zhou et al [28] developed a model for investigating the variation of flame height with pressure from the point of temperature, but they ignored the effect of species on flame structure, thus limiting their work. In this paper, a method is proposed to define different flame heights by the temperature distribution $T_1$, component $\tilde{X}$ distribution $Y_1$, and component $\tilde{Z}$ distribution $Y_3$ along the central axis of the combustion field above the AP surface as well as the axial temperature distribution $T_2$ and component $\tilde{Z}$ distribution $Y_2$ along the gas field.

Fig.10 shows the profile of the above physical quantities of SD III-22 AP/HTPB propellant at 6.89 MPa. When $T_1$ reaches 1400K [2,6], the distance from the burning surface is the AP monopropellant flame height, which is expressed as $H_1$. When $T_2$ reaches 95% of the adiabatic flame temperature under this condition and $Y_2$ is less than 0.1%, the distance from the burning surface is the primary diffusion flame height, which is expressed as $H_2$. When $T_1$ reaches 99.5% of the adiabatic flame temperature under this condition and $Y_2$ is less than 0.1%, the distance from the burning surface is the final diffusion flame height, which is represented as $H_3$. According to the above definition, these flame heights at 6.89 MPa have been marked in Fig.10, which are 1.09μm, 8.29μm, and 26.00μm, respectively.
According to above method, Table 3 shows the heights of three kinds of flame structures of AP/HTPB under different pressures. It can be seen that the heights of the primary diffusion flame and final diffusion flame of SD III-24 propellant are significantly higher than those of SD III-16 and SD III-22 under the same pressure conditions. This is because the intercept sizes of AP and HTPB of SD III-24 are relatively large, especially the AP as oxidant is much larger than others. Therefore, for the diffusion reaction $R_2$, though the fuel component $\bar{Y}$ increases, the combustion is still in the oxygen-rich environment, forming a higher primary diffusion flame and final diffusion flame. On the base of the fact affected by the physical properties of AP particles, the height of AP monopropellant flame and the content of $\bar{Y}_1$ are approximately equal for different propellants. Besides, it can be found that $H_1$ decreases and $H_3$ increases with an increase in pressure. For comparison, Fig.4 of Ref. [5] shows AP/HTPB emission images for constant binder thickness of 120-160μm with varying pressure. As pressure increases, the result shows that the overall diffusion flame appears to be widened and taller, which is consistent with Table 3 as well as the Shvab-Zeldovich theory [29]. It also shows the rationality of using temperature and components to jointly define the flame height. However, $H_3$ shows a downward trend at 0.69 MPa–10.3 MPa and remains unchanged at 13.8MPa–20.7MPa.

According to the variation of flame heights under different pressures, the pressure range of 0.69MPa-20.7MPa is divided into three regions. Taking SD III-22 AP/HTPB propellant as an example, the interval of 0.69MPa-2.07MPa is defined as region I, where the variation rates of $H_1$ and $H_2$ in this region are -1.85μm/MPa and -6.23μm/MPa, respectively. The interval of 3.45MPa-10.3MPa is defined as region II, where the variation rates of $H_1$, $H_2$, and $H_3$ are -0.06μm/MPa, -0.04μm/MPa and 1.24μm/MPa, respectively. The range of 13.8MPa-20.7MPa is defined as region III, where the variation rates of $H_1$, $H_2$, and $H_3$ are -0.01μm/MPa, 0.11μm/MPa, and 2.32μm/MPa, respectively. According to the variation rates of flame height above, the variations of $H_1$ and $H_2$ are the largest in region I and the changes in regions II and III are smaller, indicating that the AP monopropellant flame and the primary diffusion flame are close to the burning surface under high pressure. The variation rate of $H_3$ also increases with a growth of the pressure, demonstrating that the final diffusion flame controls the gas-phase combustion process of AP/HTPB propellant under high-pressure conditions.

**Fig.10.** Distribution of component $\bar{X}$, component $\bar{Z}$, and temperature

<table>
<thead>
<tr>
<th>Pressure (MPa)</th>
<th>Flame Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.69-2.07</td>
<td>Region I</td>
</tr>
<tr>
<td>3.45-10.3</td>
<td>Region II</td>
</tr>
<tr>
<td>13.8-20.7</td>
<td>Region III</td>
</tr>
</tbody>
</table>

**Table 3.** Heights of micro-flame structures of different AP/HTPB propellants
and the final diffusion flame begins to dominate the combustion process. With the increase of pressure, the chemical reaction time becomes shorter, and the diffusion process gradually becomes the dominant factor affecting the flame structure. Beckstead et al\cite{1} gave the expression of $T_d$, namely:

$$T_d = \frac{L^2}{D}$$  
(33)

where $L$ is the scale of the representative sandwich model, $D$ is the mass diffusion coefficient, where $D \propto T^{1.75}/p$.

At the same time, with the increase in pressure, the chemical reaction rate and the gas flow rate increase. The characteristic chemical time $T_c$ and characteristic flow retention time $T_f$ are described as follows:

$$T_c = \frac{\rho_g}{D_2 p^{1.7}}$$  
(34)

$$T_f = \frac{L \rho_g}{\dot{m}}$$  
(35)

where $D_2$ is the constant of the R2 chemical reaction rate, $p$ represents the gas pressure and $\dot{m}$ is the mass flow on the burning surface.

Fig.11 shows these three kinds of time scales of SD III-22 AP/HTPB propellant micro-combustion with the change of environment pressure. It can be seen that with an increase in the pressure, $T_d$ and $T_f$ increase linearly, while $T_c$ decreases rapidly. When the environment pressure is in the range of 0.69MPa-2.07MPa, $T_c$ decreases rapidly from $79.0 \times 10^{-5}$s to $33.8 \times 10^{-5}$s, the diffusion time scale $T_d$ increases from $1.6 \times 10^{-5}$s to $4.2 \times 10^{-5}$s, and $T_f$ increases from $1.2 \times 10^{-4}$s to $1.4 \times 10^{-4}$s. The large change rate of $T_c$ forms the dramatic changes of $H_f$ and $H_2$ in region I. When the environment pressure is in the range of 3.45MPa-10.3MPa, the change rates of $T_c$, $T_{id}$ and $T_i$ are $1.85 \times 10^{5}$s/MPa, $1.7 \times 10^{5}$s/MPa, and $1.6 \times 10^{5}$s/MPa, respectively. Combined with Table.5, it can be seen that the change rate of $T_i$ in this interval is not very large, so $H_1$ and $H_2$ of region II are unchanged. At the same time, the large variation rates of $T_d$ and $T_f$ indicate that the diffusion mixing rates of combustion gases decrease greatly and the final diffusion flame begins to dominate the micro-combustion process of AP/HTPB. The values of $T_c$ at 0.69 MPa are 9.65 times at 13.8MPa, 11.35 times at 17.25MPa, and 12.97 times at 20.7MPa, respectively. At the same time, the variation rates of $T_d$ and $T_f$ are $1.6 \times 10^{5}$s/MPa and $1.2 \times 10^{5}$s/MPa, which are much larger than $T_c$. On the one hand, the chemical reaction rate of region III is getting faster and faster. On the other hand, the variation rates of

<table>
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<tr>
<th>Parameters</th>
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<th>SD III-22</th>
<th>SD III-24</th>
</tr>
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<td>/</td>
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</tbody>
</table>

4.4 Effects of environment pressure on micro-flame structures

To further reveal the influence of different environmental pressures on the micro-flame, three kinds of characteristic time constants, namely characteristic diffusional time $T_d$, characteristic chemical time $T_c$, and characteristic flow retention time $T_f$, are introduced to describe the gas-phase combustion characteristics under different pressure conditions.

![Table](image-url)
$T_d$ and $T_f$ with a higher value make the diffusion mixing rates of components $\tilde{Y}$ and $\tilde{Z}$ far behind the chemical reaction rate of $R_2$, so the change rate of $H_j$ of the final diffusion flame in region III is the largest.

![Graph](image)

**Fig.11.** Characteristic parameters of three propellants under different pressures

$Pe$ and $Da$ are introduced to represent the relative size of characteristic diffusional time $T_d$, characteristic chemical time $T_c$ and characteristic flow retention time $T_f$, where $Pe = T_d/T_f$ and $Da = T_d/T_c$, as shown in Fig.11. $Pe$, which represents the ratio of convective-to-diffusive transport rates, is physically related to the burning rate and the binder thickness. $Da$, which represents the ratio of chemical reaction and diffusive transport rates, is related to the pressure and binder thickness. These two parameters are not independent, it can be seen from Fig. 12, with an increase in pressure. $Pe$ and $Da$ all show an increasing trend. Under low-pressure condition (0.69MPa–2.07MPa), it shows $0.126 < Pe < 0.28$ and $2.03 \times 10^2 < Da < 1.24 \times 10^3$. The increased diffusion mixing at small $Pe$ and $Da$ will reduce the local component $\tilde{Y}$ fraction in the overall flame region, which possibly eliminates the presence of stoichiometric regions. In addition, the influence of $Da$ becomes more subtle compared with $Pe$, affecting reaction intensity. A small $Da$ tends to form the ‘lifted flame’ reported in the literature [29] as well as the flame structure that is like that at 0.69 MPa in Fig.15. With an increase of the pressure (2.07MPa-10.3MPa), it presents $0.28 < Pe < 0.64$ and $1.24 \times 10^3 < Da < 1.77 \times 10^4$. $Da$ is significantly larger and $Pe$ is also continuing to grow in this region, the gas flame gradually attaches to the surface despite the relatively strong convection. The mixture flow begins to move away from the burning surface, references [5,29] and numerical calculation indicate that fewer oxidizing-gas (component $\tilde{Z}$) reaches the center of HTPB, thus the relatively slow reaction above HTPB causes the separation of flame. In region II, the micro-combustion process is affected by both chemical kinetics and limited fluid dynamics. The flame shows premixed-diffusion characteristic, forming the flame structure that is like that at 3.45MPa in Fig. 12. When the pressure is above 10.3 MPa (0.64 < Pe < 0.86 and $1.77 \times 10^4 < Da < 5.75 \times 10^4$). The reactants are further carried out away from the burning surface because the diffusion process becomes important even dominant, leading to a taller overall diffusion flame concentrated in the AP side, which is like the flame at 20.7 MPa in Fig. 12. All in all, the predicted trend of flame structure with $Pe$ and $Da$ in accordance with BDP model[2], experiment results of literature [5,29] and numerical result of this paper.
To further illustrate the effects of the reactants diffusion process on flame structure, the diffusion flame can be divided into two regions by leading edge flame (LEF) [30]: (1) flame front and (2) trailing diffusion flame. Based on above analysis in this paper, the interaction between diffusion mixing and chemical reaction in the gas phase of AP/HTPB combustion and the resulting flame structure can be further illustrated. That is, near the AP/HTPB burning surface, the diffusion rate between solid pyrolysis products is much faster than the chemical reaction rate due to the low temperature around the burning surface. Thus, a small region of partially premixed reactant flow develops and moves away from the burning surface under the diffusion effect, which continuously absorbs the energy from the high-temperature diffusion flame, resulting in a continuous increase in temperature. When the temperature of the premixed reactant flow approaches adiabatic flame temperature, LEF is formed, as shown in Fig.13.

The flame front is located in the gas flow where the premixed process is concentrated. The chemical reactions occur in this area, which consumes most of the gaseous reactants in the space and yields a lot of heat energy, so the gas-phase heat release core is formed in the flame front. At the same time, the larger heat release causes that the temperature of the gas mixture downstream of the LEF increases rapidly, which becomes a flame holding site for the trailing diffusion flame. Compared with the flame front, the energy of the trailing diffusion flame is lower, which is attributed to the small conductive and convective heat losses in the trailing diffusion flame.

Therefore, when the pressure is low, and $Pe$ and $Da$ are small, the gas-phase combustion is dominated by chemical kinetics. Due to the lower gas phase release, the premixed flow near the burning surface needs to absorb more energy from the diffusion flame to approach adiabatic flame temperature, forming a lower diffusion flame and higher LEF. When the environment pressure is high, the gas-phase combustion is dominated by the diffusion effect, larger $Pe$ and $Da$ results in a longer diffusion flame. Under the high temperature effect of the burning surface, the gas mixture near the burning surface is easier to reach adiabatic flame temperature, forming a higher diffusion flame and lower LEF. At the same time, with the increase of $Pe$ and $Da$, the LEF further into the AP side and away from the oxidizer fuel interface according to the literature [30], as shown in Fig. 13 (where AMF represents the AP monopropellant flame).
5. Conclusions

The current study is to develop a method to exactly evaluate the micro-combustion process of AP/HTPB propellant using a sandwich model. The two-step global kinetic reaction and one-step reaction represent the processes of gas combustion and condense-phase decomposition. The predicted average burning rates match well with the experimental cases, indicating the accuracy of the proposed model.

A series of typical combustion characteristics are examined to elucidate information on multi-flame structure emanating from AP/HTPB propellant in detail. To quantitatively explain the gas phase flame structure under different environmental pressures, a method is proposed to jointly define the AP monopropellant flame height $H_1$, the primary diffusion flame height $H_2$ and the final diffusion flame height $H_3$ by the temperature and components distribution of the gas-phase field. Meanwhile, $Pe$ and $Da$ are also introduced to illustrate the influence of chemical kinetics and diffusion mixing process on gas-phase combustion. Many important flame properties observed in the experiment can be replicated by this model, confirming the rationality of this approach and motivating further development.

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