Safety design and numerical simulation of twin screw extruder for energetic materials

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Abstract: To improve the safety performance of twin screw extruder for energetic materials, the finite element method is used to simulate the explosive moment of energetic materials in the twin screw barrels with different pressure venting structures. The explosive pressure distribution rule and the deformation of barrels are compared. The results show that the maximum pressure and maximum shear rate which can lead to explosion both appear on the top of screw flight and in the intermeshing region. When the explosion occurs in the horizontal split barrel, the second explosive pressure peak is significantly reduced and the deformation of the barrel is much smaller. In the twin screw barrel with the pressure releasing holes, two explosive pressure peaks are both high and the fixed part of barrel has large deformation. Therefore, using the clamshell type barrel can reduce the damage of equipment and improve the safety of twin screw extruder for energetic materials.

1. Introduction

With the requirements on weapons systems of wars increasing, new formulations of energetic material are appearing all the time. Traditional processing technologies do not unable to meet the requirements of multi-species, high-quality production. In the early 1970s, the developed countries began to study the continuous manufacturing process of energetic materials by twin screw extruder. And in the mid-to-late 1980s, they completed the transition from the intermittent manufacturing process to the continuous process [1-3]. In the mid-1990s, the United States, Germany, France, Switzerland and Japan had overcome the difficulties of twin screw mixing and extrusion technology of energetic materials [4-9].

From the 1990s, China began to study mixture and extrusion of energetic materials by using twin screw. The research mainly focused on the structures and process parameters of the twin screw continuous extrusion technology [10-12], which has not been widely used in the field of energetic materials yet [13].

The twin screw extruder can realize continues and flexible preparation of energetic materials. At present, there are more studies on screw structures, but less research on the safety design of barrel structures. Compared with the screw, replacement of damaged barrel requires more time and has greater difficulty in processing. At present the deformation of the material under the impact load of the
explosion is mainly studied by experiment and numerical simulation [14-16]. This paper focuses on the effect of explosion venting structure of the Φ50 twin screw extruder on the pressure distribution law and barrel deformation, and provides theoretical support for the safety design of twin screw extruder for energetic materials.

2. Analysis of the flow field in the barrel

2.1. Screw and runner model

This thesis concentrates on the design of intermeshing co-rotating twin screw extruders for energetic materials. The structure of screw contains two different thread elements. The geometric parameters of the thread elements are as follows: the external diameter of the screw is 50.4 mm, the center distance is 40.8 mm, the gap between the barrel and the outer diameter of the screw is 0.5 mm, and the pitches are 50 mm and 75 mm, respectively.

The geometric models of the screws and runners are shown in figure 1. The screws are divided by the tetrahedral elements, and the runners are divided by the hexahedral elements as shown in figure 2. The meshes of the part of screw contact with the runner are refined.

![Figure 1. Geometry models of different screws and runners.](image)

![Figure 2. Grid models of different screws and runners.](image)
2.2. Constitutive equation of fluid
According to the experiment result of energetic materials substitute, Bird-Carreau model is chosed to describe the flow characteristics in the runner. The relationship expression of shearing viscosity and shearrate is as below:

$$\eta(\dot{\gamma}) = \eta_0 + (\eta_0 - \eta_\infty)(1 + \lambda^2 \dot{\gamma}^2)^{(n-1)/2}$$

The rheological parameters of material are shown in table 1.

**Table 1.** The rheological parameters.

| $\eta_0/10^4\text{Pa} \cdot \text{s}$ | $\lambda/\text{s}$ | $n$ | $\eta_\infty/\text{Pa} \cdot \text{s}$ |
|-----------------------------------|------------------|-----|-------------------------------------|
| 2.62                             | 1.86             | 0.12          | 2.96                                |

2.3. Boundary condition
Considering that the actual mixture and extrusion experiment adopts the measuring feeding technology, we should set the constant flow entrance condition, and the boundary condition of the outlet should be constant pressure. All boundary conditions are shown in table 2.

**Table 2.** Boundary conditions.

| Boundary                        | Condition           |
|---------------------------------|---------------------|
| Inner surface of the barrel     | $v_w=v_r=0$         |
| Screw speed                     | 20 r\cdot\text{min}^{-1} |
| Inlet flow                      | 3.33×10^{-6} m\cdot\text{s}^{-1} |
| Outlet pressure                 | 0 MPa               |

2.4. Analysis of simulation result
If the energetic material is greatly stimulated in the manufacture process, there is a high probability of explosion. So, in all the flow field parameters, the pressure and shear rate in the mixture runner have greatly effect on the safety performance. When the pressure or the shear rate is high, the energetic material is easy to be ignited, which will lead to explosive.

**2.4.1. Pressure distribution in the runner.** The pressure distribution in the runner is shown in figure 3. Figure 3 (a) and figure 3 (b) show the difference of pressure contours between 50/50 specification and 75/75 specification threaded elements.
Figure 3. Pressure distribution in runner.

It can be seen that compared to the 50/50 specification threaded element, the 75/75 specification threaded element can produce more pressure in the runner, and maximum pressure on the material increases by 2.21 times. Comparing the pressure contours in the figures, it is observed that the maximum pressure on the material is found on the top of the screw flight and in the intermeshing region.

2.4.2. Shear rate distribution in the runner. The shear rate distribution in the runner is shown in figure 4. Figure 4 (a) and figure 4 (b) are the shear rate contours in the runners of 50/50 specification threaded element and 75/75 specification threaded element, respectively.

Figure 4. Shear rate distribution in runner.

As can be seen from figure 4, compared with the 50/50 specification threaded element, the 75/75 specification threaded element produces a slightly higher shear rate. Similar to the pressure contour,
the high shear rate areas appear on the top of the screw flight and in the intermeshing region.

3. Safety analysis of barrel structure

3.1. Barrel model

The ordinary barrel is shown in figure 5(a). There are two explosion venting structures which are used frequently now. Structure one as shown in figure 5 (b) is the horizontal split barrel, Structure two as shown in figure 5 (c) is the barrel with two pressure relief holes.

![Barrel models](image)

Figure 5. Barrel models.

Since we focus on the damage to the barrel caused by the shock wave, the screw is simplified to a cylinder, and the runner is semi-full of fluid. In the barrel, there are 1035 g TNT, and the remaining part of the barrel is filled with the ideal air under the standard atmospheric pressure, as shown in figure 6. All parts are divided by the hexahedral elements.

![Diagram of screws and barrel simplification structures](image)

Figure 6. Diagram of screws and barrel simplification structures.

3.2. Material parameter

The barrel and screw are made of 45# steel which has excellent performance. The material parameters of the steel are shown in table 3 and material parameters of TNT are shown in table 4.
Table 3. Material property of 45# steel.

| Property                             | Value |
|--------------------------------------|-------|
| Yang's modulus (GPa)                 | 209   |
| Poisson ratio                        | 0.269 |
| Yield limit (MPa)                    | 355   |
| Tangent modulus (GPa)                | 2.09  |
| Tensile limit (MPa)                  | 600   |

Table 4. Material property of TNT.

| Property                             | Value |
|--------------------------------------|-------|
| Density (kg/m³)                      | 1630  |
| Detonation velocity (m/s)            | 6930  |
| Energy density (kJ/m³)               | 6×10⁶ |
| Detonation pressure (GPa)            | 21    |

3.3. Constraint and load condition

The bottom of the barrel (a) is connected to the equipment base which is considered as a fixed constraint. The upper half of the barrel (b) is fixed, and the lower half is resisted by the hydraulic system. The barrel (c)’s bottom is fixed on the base of the equipment and has two pressure relief holes at the top. The discharging pressure is 10MPa.

According to the simulation results in section 2.4, on the top of the screw flight and in the intermeshing region are easy to incur explosive accidents and the detonation point locations. Autodyne is used for explosive simulation calculations and to record changes in pressure over time.

3.4. Change of pressure

3.4.1. Change of pressure in the barrel. The curves of the pressure in the barrels versus time when the detonation points are on the top of the screw flight are shown in figure 7 (a), and the curves when the detonation points are in the intermeshing region are shown in figure 7 (b).

![Figure 7 Curves of pressure in the barrel versus time](image)

As can be seen from the p-t curves in figure 7 (a), when explosive happens on the top of the screw flight, the pressure in the barrel rises instantaneously. At 0.01 ms, the pressures in the barrel (a), (b), and (c) all raise to about 9100 MPa. In the barrel (a), after the initial impact, the shock wave is reflected by the inner wall of the barrel and screws, which produces the secondary impact.
reflection caused a significant secondary pressure peak on the curve which is lower than the first time. Due to the action of explosion venting structure, there is no secondary pressure peak in the p-t curve of the barrel (b), while the secondary pressure peak of the p-t curve of the barrel (c) is slightly lower than that of the barrel (a).

As can be seen from the p-t curves in figure 7(b), when the explosive happens in the intermeshing region, the initial pressure peaks in the barrel (a) and (c) are about 7000 MPa, the pressure curves both have a significant secondary pressure peak, while the initial pressure peak in the barrel (b) is lower which is 6195 MPa, and there is no secondary pressure peak.

3.4.2. Change of pressure on fixed part of barrel. The curves of the pressure on the barrel fixing part versus time when the detonation points are on the top of the screw flight are shown in figure 8 (a), and the curves when the detonation points are in the intermeshing region are shown in figure 8 (b).

![Figure 8. Curves of pressure on the barrel fixing part versus time.](image)

As can be seen from the curves in figure 8 (a), when explosive happens on the top of the screw flight, the initial peak of pressure curve of barrel (a) appears at 0.01 ms, and the maximum pressure appears at 0.025 ms which is 4727.2 MPa. The pressure curve peaks of barrel (b) and barrel (c) are both appear 0.015ms, and the values are 3578.6MPa and 4358.8MPa, respectively. At 0.07 ms, the pressures of barrel (c) increase, and the pressure peak reappeared. The pressure on the barrel (b) is the lowest.

As can be seen from the pressure curves in figure 8 (b), when the explosive happens in the intermeshing region, the pressure peaks of curves all appear at 0.005 ms, which are about 5500 MPa. After that, the pressures decrease, and the pressure peaks reappear at 0.03 ms. At 0.065 ms, the pressure on fixed part of barrel (a) increases to 3536.4 MPa. At 0.07 ms, the pressure on fixed part of barrel (c) increases to 3915.8 MPa, while the curve of barrel (b) does not rise.

Based on the above analysis, we can see that compared with the ordinary barrel, when the explosive happens in the horizontal split barrel, the pressure in the barrel and on the fixed part both decrease, and there is no secondary pressure peak. When the explosive happens in the barrel with two pressure relief holes, both pressures have little change, and the secondary pressure peak just slightly reduces.
3.5. Deformation of barrel fixed part

3.5.1. The detonation points on the top of the screw flight. The curves of the deformation of the barrel fixed part versus time when the detonation points are on the top of the screw flight are shown in figure 9. The deformation contours of fixed part of barrel (a), (b) and (c) at 0.03 ms and 0.06 ms are shown in figure 10, figure 11 and figure 12, respectively.

![Figure 9. Curves of barrel fixed part deformation versus time.](image)

As seen in figure 9, when explosive happens, the deformation of the barrel (a) increases rapidly, and the first peak occurs around 0.03 ms. Under the action of secondary impact, the deformation reaches the maximum value at about 0.06 ms. The fixed part of barrel (b) has the largest deformation around 0.025 ms, and then the deformation decreases gradually. On curve of barrel (c), the first peak appears around 0.025 ms, which is relatively flat. There are two consecutive large deformations around 0.65 ms and 0.75 ms, which indicate that the impact of the explosion has not been effectively relieved.

![Figure 10. Deformation contours of fixed part of barrel (a) (magnified 2 times).](image)
Figure 11. Deformation contours of fixed part of barrel (b) (magnified 2 times).

Figure 12. Deformation contours of fixed part of barrel (c) (magnified 2 times).

Compared figure 10 figure 11 and figure 12, we can see that the fixed part of the barrel (a) appears significant deformation. Although the maximum deformation of the fixed part of the barrel (c) is smaller than that of the barrel (a), compared with the barrel (b), the deformation is still very obvious.

3.5.2. The detonation points in the intermeshing region. The curves of the deformation of the barrel fixing part versus time when the detonation points are in the intermeshing region are shown in figure 13. The deformation contours of fixed part of barrel (a), (b) and (c) at 0.03 ms and 0.06 ms are shown in figure 14, figure 15 and figure 16, respectively.

Figure 13. Curves of barrel fixed part deformation versus time.

As seen in figure 13, the deformation of the barrel (a) increases rapidly after explosive. The first
peak occurs at about 0.03 ms. Under the action of secondary impact, the deformation reaches a large value at about 0.065 ms. The barrel structure of the intermeshing region is relatively thin, so the initial impact of the explosion in this area has a greater effect on the barrel.

The fixed part of barrel (c) has the largest deformation at about 0.02 ms. And then the deformation reduces gradually but getting larger from 0.05 ms to 0.085 ms. The maximum deformation of the fixed part of barrel (b) appears at about 0.03ms. The deformation curve is flat, indicating that the impact of the explosion has been effectively relieved.

As shown in the figures, the fixed parts of barrel (a) and barrel (c) are significantly deformed. Compared to the barrel (a), the maximum deformation of the barrel (b) is reduced by 43.2% and the
barrel (c) is 3.8% less only.

Based on the above analysis, we can see that compared with the ordinary barrel, when the explosive happens in the horizontal split barrel, the deformation of fixed part significantly reduces, and the changes in deformation over time is fewer. When the explosive happens in the barrel with two pressure relief holes, the deformation is slightly reduced, and there is a significant secondary impact effect, which leads to a large deformation.

4. Conclusions

(1) In the process of energetic material production by twin screw extruder, the maximum pressure and shear rate appear on the top of the screw flight and in the intermeshing region where are easy to incur explosive accidents and the detonation point locations.

(2) Compared with the ordinary barrel structure, the pressure in the horizontal split barrel is obviously reduced. Since the barrel is opened by shock wave, the secondary pressure peak disappears, and the deformation of the fixed part of the barrel decreases significantly.

(3) Compared with the ordinary barrel structure, the reduction of pressure in the barrel with two pressure relief holes is not obvious. Under the effect of the two shock waves, the barrel has a large deformation.

(4) Using the twin screw extruder with the horizontal split barrel to produce energetic materials can reduce the damage to the barrel in an accident and improve the safety performance.

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