Mechanics model and optimum design of PE pellet shell for anti-water-seepage with ease in open

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Abstract. Polyethylene capsule shells are a kind of container for pills with low cost and long-term preservation, after paraffin-sealed. This kind of pellet shell is composed of two hemispheric shells with the seal convex and concave allowances, at which they connect, locate and unify together as a whole by local elastic deformation. However, the water seepage occurs in certain percentage of the pills during paraffin-seal operation. In order to solve the problem of water seepage and further improve the process, the current study presents the tension model under the action of ideal gas in paraffin-sealing, the enhanced cantilever beam model under water cooling, and the simply supported beam model for investigation of the cause of the water seepage. The criterion of impervious water was put forward and developed with anti-inference method. The case analysis shows that the seepage is caused by the unreasonable structure of the seal of PE pellet. On the basis of this, the seal allowance of the shell is improved and optimized in the current design. And the overlap amount of the half shells was increased from 0.15mm to 0.30mm, at least, with protruding and half shot shell with concave is increased and the small angle of the double V structure is adopted. The results of calculation and test show that the new design is of rational and reliability, and it met the requirements of small force and ease in opening the shell.

1. Introduction
Polyethylene (PE) pellet shell design and manufacture for storage of pill are supposed to ensure that there are no cracks, uniformed wall thickness, no material defects, no dis-colour, with even mating surfaces, and tightness after paraffin seal [1, 2]. The main stages of the existing production process is ingredients, injection molding, shell test, filling the pellet with a pill, paraffin seal, test and inventory [3, 4]. Among them, paraffin seal is the key technical link of storing quality, packing transportation and sales of proprietary drugs in the pellet, and the key issue is good tightness. A kind of PE pill shell made by a certain enterprise was found to have leakage during the paraffin sealing. After the process examination, the original design was considered to be a problem, and the preliminary calculation and test also showed that the original design was not reasonable, resulting in water leakage. The synthesis of the pellet shell depends on the elastic deformation of the joint surfaces and then encapsulated by
paraffin, as shown in figure 1. The existing pill shells have structure of v-type joint and paraffin seal preservation, and there are many studies on the formulation and properties of polymer packaging shell materials [5-8]. However, there are few reports on the mechanical deformation and sealing technology in the paraffin seal process of PE[9,10].

In the current study, the stress and deformation of the paraffin seal of PE pellet shells were analyzed in detail, and the corresponding mathematical models of the force and deformation of the pellet shells were put forward and developed. The cause of water seepage was investigated and revealed combined with the criterion of no water seepage. A case study showed that the mathematical models proposed in this paper are applicable, and the new design met the requirements of impervious water and easy opening.

**Figure 1.** State and paraffin-sealing of the polyethylene pellet

(a) two halves of the shell; (b) unification of the two halves; (c) paraffin-seamed shell

2. Material properties and shell requirements

2.1. Some physical properties of PE material

Drug packaging materials, especially those directly in contact with drugs, play a decisive role in ensuring the stability of drugs [12-14], so the applicability of materials will directly affect the safety of drugs. PE is one of these materials used for this purpose. Some basic properties of the PE material is shown in Table 1. Polyethylene (chemical formula : (C2H4) N ) is a thermoplastic resin made by polymerization of ethylene, which includes a copolymer of ethylene with a small number of α-olefin. Polyethylene is odourless, non-toxic, feels like paraffin, and has good low temperature resistance (the lowest temperature can reach -100 ~ -70 ℃), chemical stability is good, and is resistant to most of acid and alkali erosions. It is insoluble in ordinary solvents at room temperature, less water absorption, excellent electrical insulation.

**Table 1.** Some of the PE properties

| Style of point Concentration | Value of Concentration g/mm³ | Coefficient of linear expansion ×10⁻⁵/K | Elastic module N/mm² | Tension stress N/mm² | Melting °C |
|-----------------------------|-------------------------------|----------------------------------------|----------------------|----------------------|------------|
| High                        | 0.000941-0.000965             | 20-24                                  | 1072                 | 22.1                  | 140        |
| Middle and low              | 0.000910-0.000940             | 20-24                                  | 172                  | 13.27                 | 140        |

2.2. Requirement of the pellet

The pellet made of polyethylene will be produced into a spherical shell with two halves of radius 13mm, wall thickness 1mm, housing the pill of radius 8mm; the thickness of seal allowance ≤2.0mm; paraffin-sealing at 70 ℃ is done without water seepage; opening the pellet is with ease after paraffin-sealed, and the opening force is less than 5kgf.
3. Paraffin seal process and mechanical models

In order to quantitatively analyze the force and deformation of the pellet during the encapsulation of the pellet shell, and then determine the gap and size of it, it is necessary to build the corresponding mathematical model and analyze it in detail.

3.1. Analysis of paraffin sealing process

The paraffin dipping process is completed for the shells to dip in liquid paraffin at a higher temperature after the two half shells are buckled. The temperature change in this process was observed. The pellets and pills were at room temperature (or a specific temperature). After the dip is completed, the water is cooled and removed from the tank. The capsule shells have experienced cleaning, storing the pill into a shell, unification of the two half shells, and paraffin-sealing. At the same time the gas in the capsule pellet experiences the room temperature, through dipping in paraffin temperature, and cooling to back to the room temperature. The pellet shells, during the above period have stress balance between the inside and outside of the shells, followed by stressed with the gas heat expansion, and both inside and outside forces become to meet the new balance in cooling phase formation pressure difference inside and outside temperature difference, Eventually, temperature difference between inside and outside the pellet turns to zero, and the stress reaches a new balance. The water seepage occurs at the stage of cooling and the formation of pressure difference comes out with the temperature.

3.2. The ideal gas equation in process of paraffin sealing

We regard the gas in the pellet shell as ideal gas before, during, and after, the dipping of the paraffin and investigate the influence of temperature change on the force exerted on the pellet shell. According to the ideal gas formula, we have

\[ PV / T = P_0 V_0 / T_0 \]  

\[ PV / T = (m / M)RT \]  

From equation(2), the pressure on the inner surface of the pellet is

\[ P = P_0 \times V_0 \times T / (T_0 \times V) = \nu(P_0 \times V_0 \times T / (T_0 \times V)) = (m / M)RT / V \]

3.3. Strengthened cantilever beam deformation model and impervious criterion

The spherical shell end expands outwards under the action of internal tension. The half shell with the convex seal allowance is impeded by the half shell with the convex seal allowance. Under the action of internal tension, it can only make closer contact with the half shell with concave seal allowance, that is, there is no tendency to water seepage. So it was not considered in checking the water seepage by calculation of the displacement of the convex seal allowance. The half-shot shell with the concave seal allowance expands under the action of tension relatively to the counterpart of the shell, and does possess a certain tendency of free opening. When the displacement reaches a certain value, water seepage will occur. Therefore, we concentrate on this displacement. Because of hemisphere shell morphology with half A bolus of the concave shells have bigger difference, curved beam and straight beam is to simplify and abstract in order to strengthen cantilever beam, cantilever beam on the fixed end of mouth vertical distance as the vertical plane of point C, e concentrated tension P in free endpoint. A, strengthen support and cantilever form isosceles right triangle, cantilever and supporting for rectangular section A, as shown in figure 2.

**Figure 2.** Cantilever model and force analysis of the shell in paraffin seal cooling
The free end A is taken as the reference point on the half shell with concave seal allowance mating with the half shell with convex seal allowance. In the deformation process of AC with tension and AB with compression, point A moved to point $A'$ through the horizontal elongation of $\Delta L_{AC}$ and the vertical compression of $\Delta L_{AB}$.

3.3.1. Deformation of the seal allowance in seal cooling with paraffin seal. The deformation of the shell during the paraffin seal process is caused by the internal tension under the pressure difference between the inner and outer shell. Pressure difference is

$$\Delta P = P - P_0 = \frac{(m/M)RT}{V} - P_0$$  \hspace{1cm} (4)

So, the tension on the half shell with concave seal allowance is

$$F = \pi (R^2 - r^2) \Delta P / 2 = \pi (R^2 - r^2) \frac{(m/M)RT}{V} - P_0) / 2$$  \hspace{1cm} (5)

Equation (5) may be thought as the concentrated force exerting on the free end of the cantilever, according to the mechanical model in figure 2. Due to the apparent difference between the hemispheric shell and a straight beam, the half shell is simplified and abstracted as strengthened cantilever beam, as shown in figure 2. The fixed end of the cantilever beam is at a plane perpendicular to the beam with distance of $e$, and the concentrated tension $P$ acts on the free end. The reinforced support bar, the cantilever and BC form an isosceles right triangle, with rectangular section A. The force $P$ acting on the half shell with concave seal allowance may be decomposed according to the parallelogram rule, and the two components are horizontal force $P'$ and supporting force $P''$, respectively. The horizontal force $P'$ makes the bar AC extensile while the supporting force $P''$ let bar AB compressive. It is known that $P = F$ and $E$ is the elastic modulus of the pellet material ($E_1$ is the elastic modulus of the low-medium density and $E_2$ is the elastic modulus of the high-density). Assume that the section shape of the cantilever beam is the same as that of the reinforced support section, with the cross-section area, A, and the supporting angle is $\theta$. Then we have

$$P' = P \tan \theta$$  \hspace{1cm} (6)

$$P'' = P / \sin \theta$$  \hspace{1cm} (7)

Bar AC is subject to tension while that of AB to compression.

$$\Delta L_{AC} = \frac{(P')/A}{(AC/E)}$$  \hspace{1cm} (8)

$$\Delta L_{AB} = \frac{(P'')/A}{(AB/E)}$$  \hspace{1cm} (9)

In the right angled triangle, $\Delta A'A''$, $\angle A'A'' = \theta$, we have

$$\Delta P = A'A'' = \Delta L_{AC} \tan \theta = \frac{(P')/A}{(AC/E)} \tan \theta = eP \tan^2 \theta / E$$  \hspace{1cm} (10)

3.3.2. Criterion of impervious sealing of the paraffin sealed pellet. In theory, water seeps through the gap. Before the paraffin sealing operation whether the pellet is water seepage nor depends on the geometry of the mating joint. After the paraffin sealed it is determined with the displacement of the two half shells by pressure difference between the inner and outer shell. As long as the actual overlap amount of the pellet is less than zero, water seepage occurs. That is

$$\Delta P - \Delta > 0$$  \hspace{1cm} (11)

where $\Delta P$ is displacement of half shell with the concave seal allowance on mating surface after paraffin seal. The seal allowance expands outwards under the action of internal tension, and the half shell with convex seal allowance is hindered by the shell with concave seal allowance. As a result, it can only contact the half shell with concave seal allowance and make the gap (if there is one) even smaller. There is no tendency of water seepage from the half shell with convex seal allowance, so it is not considered. The half shell with concave seal allowance expands under the action of tension, and if the displacement relative to the half shell with convex seal allowance appears, and possibly, the displacement quantity exceeds the overlapping value, water seepage will occur. Therefore, we only need to check and calculate the displacement of the half shell with seal allowance in a conservation way. From equations (10) and (11), we have
\[ eP \tan^2 \theta / E - \Delta \leq 0 \]  

Equation (12) is the criterion of no water seepage after the paraffin seal.

3.4. The deformation model of simply supported beam for opening of the pellet

When opening the paraffin sealed shell (pill), it is hopeful to save effort, that is, the pinching force is not greater than a certain value (say 5 kgf). On the macroscopic view, the pellet is a spherical before it is exerted by pinching, and becomes of ellipsoid, as shown in figure 3. The stress and deformation analysis is as follows: Before pinching, the shell was not subjected to obvious external force (self-weight neglected), so the original state of the shell was maintained as a sphere shell. See figure 4. Two points A and B on the shell are on the surface of the sphere. With the application and continuous increase of pinch force S, the two half-pellet shells undergo elastic deformation at the same time. The points A and B on the spherical surface are shifted to the points A' and B' on the ellipsoid surface, respectively. At this moment, if the overlapping value of the two half shells on the mating surface, \( \Delta \), is less than zero, that is \( \Delta < 0 \), the pellet opens. We focus on the two limit states of "original" and "open" without considering the intermediate detail. Therefore, we make an abstraction, regarding the original A B as a straight connected rigid body, and we move the rigid body to A'B' position through pinching. Similarly, we can simplify and abstract again, moving point B to point B' ——— the displacement of point B in the vertical direction ——— AB is converted to A'B'. BB' is take then from the greatest deflection of the beam.

Therefore, the pellet shell that is easy to be opened on the premise of non-permeable water is carried out for deformation according to the anti-inference method, that is, the displacement of the pellet shell is first calculated and determined, and then the additional concentrated load corresponding to the deformation of the pellet shell is analyzed so as relationship between the deformation and the pinching force S may be obtained, with the help of the simply supported beam model. The main specific process is as follows: normally open the pellet is with the pinch on the seam allowance of corresponding 180 degrees of the two positions of D and D' from each other, and the pill opening position corresponding to D and D' turns 90 degrees from points of E and E', as shown in figure 7.

Indeed, the calculation of the pellet opening runs with the computation of the relative displacement on the mating surface between the convex half shell and the concave half shell. If such displacement is greater than the overlapping value, the pellet will open. In other words, if the mating condition is in failure, the pellet then will open, as shown in figure 3 and figure 4. By simply supported beam maximum deflection formula, we have

\[ f_{\text{max}} = SL^3 / (48EI) \]  

Then we have

\[ BB' = SL / (4EI) \]  

where \( f_{\text{max}} \) —— the maximum displacement; \( S \) —— the opening force; \( I \) —— inertia moment of the beam; \( L \) —— effective length of the beam. The displacement of the seal allowance along the opening direction is
$AA' = A'O - d / 2 = (AB^2 - OB^2)^{1/2} - d / 2 = [(\sqrt{2}d / 2)^2 - (d / 2 - SL^3 / (EI))^2]^{1/2} - d / 2 \quad (15)$

Let the above equation be equal to the amount of overlap, we obtain a minimum opening force, $S_{MIN}$:

$$S_{MIN} = \{d / 2 - [d^2 / 2 - (\Delta + (d / 2)^2)]^{1/2}\} 48EI / L^3 \quad (16)$$

4. Quantitative analysis of shell mechanics and deformation for improved design

4.1. Conditions and basic parameters

The PE pellet with the diameter of 26mm and the wall thickness of 1mm was taken as an example for quantitative analysis, as shown in figure 6. The force and deformation of the pellet during the paraffin sealing process were specifically investigated to find out the cause of water seepage, and then the design was improved and optimized to achieve the goal of impervious water and easy opening of the pill.

4.2. Calculation of mechanical deformation of the pellet

The volume of internal air after sealing, pressure and room temperature can be calculated and pressure $F$ inside the capsule at 70 degrees Celsius will be got

$$F = 3/4 \times 3.14 \times (R^3 - r^3) = 2863.68 \times 10^{-9} \text{(m}^3\text{)}$$

$F = 4.69744 \text{(N)}$

4.3. Seepage test of paraffin-sealing operation

If the half shell with the concave seal allowance expands by more than 0.15mm relative to the half-shell with the convex seal allowance under the tension, a gap may occur and water leakage becomes inevitable. We take a close look at it and check. Bar AC is in tension while bar AB is in compression. By calculation, we have $X = 12.5557(0.0557) \text{mm}$ and $Y = -0.2254(0.2254) \text{mm}$. The displacement in the $y$ direction is the instantaneous deformation of the half shell with the concave seal allowance, so there will indispensably be a certain percentage of the pellets in water seepage.

4.4. Calculation of the opening force

Only when the displacement of the half shell with the concave seal allowance is equal to or greater than 0.45mm along the horizontal external displacement, the pellet shell will open. In fact, when the joint is held, both concave and convex seal allowances will be subjected to the extension and deformation. As a result the pellet becomes ellipsoid shell from the spherical one. Therefore, the horizontal outward displacement of the concave seal allowance is set in about 0.60mm, then no water seepage is guaranteed with easy open.

$$f_{max} = 0.61 \text{mm}; S = 2.085 \text{N}$$
4.5. Improved and optimized design
The original design runs with water seepage problem in a certain percent of the pills and with approximate opening force. We take two ways to ensure water impermeability: (1) increase the overlapping value to within 0.3-0.60mm between the half-shell with the concave seal allowance and the half-shell with a convex seal allowance; (2) adopt the double-triangle joint structure, see figure7. The minimum overlap value after improvement is 0.30, ensuring no water seepage with the minimum open force of about 3N.

5. Conclusion
The paraffin sealing process of PE pellet consisting of two half shells was analyzed, and the state of the pellet shell was studied and abstracted in the process of heat sealing, water soaking, and cooling. The ideal gaseous equation, the enhanced cantilever beam, and the simply supported beam were proposed and used to describe and analyze the forces and deformation of the pellet during the process. A sample of the PE pellet with diameter of 26mm and wall thickness of 1mm has been given by adopting the ideal gaseous equation, models of the enhanced cantilever beam, and the simply supported beam into the paraffin sealing process. In the previous design of the pellet shell, the smallest value of overlapped seam allowance is 0.15mm and the relative displacement of the half shell with the concave seam allowance is 0.2254mm. In this case it is indispensable for the pellet to seepage. An improved and optimized design is proposed, which adopted the coalescence of a small triangle and a double V shape structure. Meanwhile, the overlap amount of the pair of half shells is appropriately increased to 0.30mm at least. The experimental results show that this structure completely solves the water seepage problem of some pills and meets the requirement of easy opening of the pellet by less than 5N.

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