Mathematics Analysis and Approaches Exploration

Title: 500 mg Paracetamol tablet and optimization of its two different shapes

Statement of task: What optimized dimensions would provide the least surface area for each of the two differently shaped 500 mg paracetamol tablets? How close are the optimized dimensions of two different tablets to the actual values or to one another?

Page count: 16 pages

Introduction:

In today's world, medication has become an integral part of health care services. Many lives are saved by the right dosage of million types of different medicine. It was interesting to me how these medications are made and what standard protocols are followed in the process. However, I also thought to myself why are there differently shaped tablets for the same dosage of the same medicine. I wondered if despite their shape differences they still have similar surface areas. These thoughts led me towards being curious about the ideal surface area for tablets. Ideally the lower the surface area of the tablet, the more comfortable it would be to swallow it, especially for children. However, do pharmaceutical companies consider this factor while producing tablets? To investigate this idea, I decided to work on two different shapes of the tablet 500 mg Paracetamol (acetaminophen) and find the dimensions that would give the minimum surface area in each case and compare these values. Such comparison would give insight about the differences in surface area of the two tablet shapes and allows one to find out which tablet is easier to swallow. The two shapes are: round cylindrical and capsular.

For each shape, firstly a constraint formula is derived which is used to simplify the objective formula. Once, the surface area formula is derived, different methods of optimization and the limitations of the function domain and range will be discussed and using these methods a value for either local maxima or minima is found. Finally, the optimum dimensions of the shape would be calculated. This process is carried out twice, once for each tablet shape. Then the obtained dimensions would be compared to the original values.

The methods of optimization:

Regardless of the shape of tablet, it is important to obtain a function for surface area of the shape, also referred to as the objective function. This function can then be used to determine whether the function for surface area of each tablet is continuous or not. This is because continuity can help choose the most efficient optimizing techniques. According to Paul Dawkins, there are three methods of optimization, namely finding absolute extrema using Extreme value theorem, first derivative test, and second derivative test.

Firstly, the Extreme value theorem can be applied to a function that has a closed interval [a,b] and is continuous. When these conditions are fulfilled, it can be derived that the function has global minimum and maximum at [a,b].Local minimum and maximum can also be found at the turning points. It is also possible that in some cases, local minimum or maximum is also global (Renze and Weisstein).

The alternative optimization method is first derivative test. Using this method, critical points can be found where the first derivative of the function is 0. In other words, there is no rate of change for the variable r, the radius of the medicine pill at these points. Sign diagrams can then be drawn to discover the regions where the function is increasing or decreasing. Using these diagrams, the local maximum or local minimum can be found at a particular radius. This method is not restricted by continuity (Dawkins).

The third method, involves finding the derivative of the first derivative in order to obtain the second derivative. The new function $f''(a)$ can allow one to find the local minimum and maximum. If $f''(a) < 0$ then the function is concave down at r = a, indicating the presence of a local minimum. On the other hand, if $f''(a) > 0$ then the function is concave up at $r = a$, indicating a local maximum (Dawkins).

Discussing the limit of the functions to be obtained:

The first tablet is cylindrical in shape; therefore, the dimensions that need to be minimized are the radius and the height of the round cylinder. These could be referred to as r and h respectively. Prior to obtaining the surface area function in respect to changing radius value, it is important to discuss the limit of the function. One can derive a function directly relating surface area and radius. Then, the value of r can be used to find h. However, the dimensions of the tablet cannot be negative values, nor 0. Hence, we could say r can extend from$]\, 0, +\infty\, [$. The value for surface area cannot be negative or 0. Similarly, the acceptable range for the functions would be $]\, 0, +\infty\, [$.

The second tablet is capsular in shape. One can divide the shape into a rectangular prism with half a round cylinder attached to each end. The required dimensions are length, breadth, radius, and height. These could be referred to as l, b, r, and h respectively. Similar to the previous tablet, it is possible to derive a formula for surface area that is in direct relation to r. This implies that in order to do so, the other three variables should be defined in terms of r using constraint formulae. However, even for this case it is evident that the dimensions of the tablet cannot be negative values, nor 0. Hence, we could say r can extend from$]\, 0, +\infty\, [$.

Round cylindrical tablet:

Obtaining the function

First, in order to calculate optimization for the round 500 mg paracetamol, the volume of the tablet is required. This is because the volume is a fixed value and can be used as a constraint.

The volume of a round cylinder has the formula $V = \pi r^2 h$. To enable calculation of volume, the radius and the height of the tablet, as annotated on figure 1 and 2 below, should be measured.

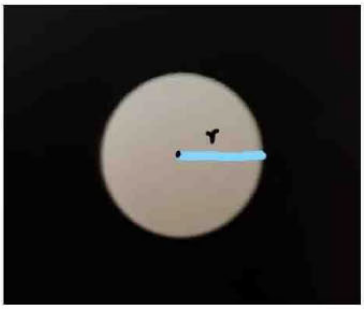

Figure 1: top view of the tablet taken by the candidate, edited using windows photos

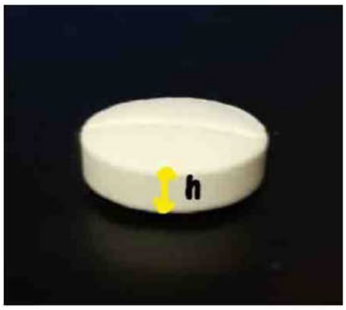

Figure 2: side view of the tablet taken by the candidate, edited using windows photos application

The measured values are r= 1.20 cm and h= 0.30 cm

The surface of the pill is curved. Therefore, a direct use of ruler is not an appropriate for taking these measurements; instead, a long thread is used to spread across the surface. Then this section of thread, representing the dimension of the pill, is measured using a ruler.

These values are then substituted in the constraint volume formula:

$$V = \pi\,(1.20)^2\,(0.30) \approx 1.36\,cm^3$$

The optimization is being done to find the minimum possible surface area. Therefore, let *SA* be surface area (cm^3), the objective function:

$$SA = \pi r^2 + \pi r^2 + 2\pi rh = 2\pi r^2 + 2\pi rh$$

We could use the constraint volume formula to derive an expression for $2\pi rh$:

$1.36\,cm^3 = \pi r^2 h$

$2\pi rh = 2\,(\pi r^2 h/\,r) = (2.71)/\text{r}$

Then we replace this value in the formula for SA:

$$SA = 2\pi r^2 + (\frac{2.71}{r})$$

Choosing the suitable optimization method based on continuity:

The equation $SA = 2\pi r^2 + (2.71/r)$ has a break at $r = 0$. In other words, there is an essential discontinuity at that specific r value. Therefore, it can be said that the function is discontinuous at $r = 0$ because $\lim_{r\to 0}\left(2\pi r^2 + \frac{2.71}{r}\right)$ does not exist.

Since the function is not continuous for $r \in IR$ and there are no closed intervals, the Extreme value theorem cannot be accepted either.

On the other hand, it is possible to try the first derivative test:

$\frac{dSA}{dr} = 4\pi r - (2.71 / r^2) = 0$

$4\pi r = 2.71 / r^2$

$4\pi r^3 = 2.71$

$r^3 = 2.71 / 4\pi$

$r = 0.600\ cm$

Here for better illustration, a table is shown instead of a sign diagram:

Interval	Testing in the function
r >0.600 cm, let r = 2	$\frac{dSA}{dr} = 4\pi(2) - (2.71/(2)^2)$ = 24.4 cm
r < 0.600 cm, let r = -2	$\frac{dSA}{dr} = 4\pi(-2) - (2.71/(-2)^2)$ = -25.8 cm

Table 1: The values of r at specific intervals

The calculations in table 1 show that the r values less than the critical point r = 0.600 cm are negative, meaning that the function is decreasing. On the other hand, the ones more than r – 0.600 cm are positive, meaning that the function is increasing at these points. Therefore, it is possible to derive that there is a local minimum at r = 0.600 cm.

It is important to mention that negative r values in the interval] -∞, 0 [were only used in table 1 for the purpose of the first derivative test and it is well-accepted that the surface area function is limited to] 0, +∞ [due to restrictions previously outlined.

The local minimum can be further confirmed using the second derivative test which is also possible for this function because no continuity requirement exists.

$$SA'(2.71) = 4\pi + (2.714336/r^3) = 4\pi + (2.714336/((0.60))^3) = 25.1$$

Second derivatives of SA > 0 therefore SA has local minimum at $r = 0.60\ cm$

The graph of the function that supports all above statements is provided in figure 1 below:

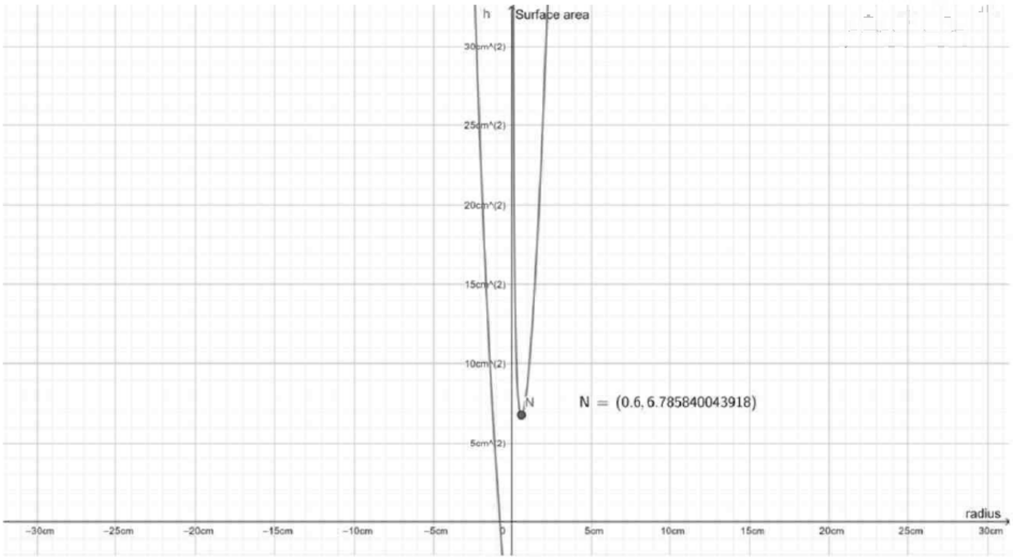

Figure 3 : Graph of the function: $SA = 2\pi r^2 + \frac{2.71}{r}$ with k showing the coordinate for the local minimum- drawn by candidate using the GeoGebra software

Having explored all the possible methods for the optimization of this shape, it is possible to reflect that the first derivative test along with sign diagram is the best method for this case because it can determine the local minima and maxima, as well as the nature of the graph at certain r values: increasing or decreasing. The second derivative test on its own is not suitable for the purpose of this optimization problem because it is dependent on the first derivative test for its outcome and the x coordinate of the local minimum is required.

Finding all optimized dimensions:

The height (*h*) of the cylinder can be found in this manner:

$$2\pi rh = \frac{2.71}{r}$$

$h = \frac{2.71}{2\pi r^3} \approx 2.00$ cm

Capsular tablet:

Obtaining the function

First, in order to calculate optimization for the capsular 500 mg paracetamol, the volume of the tablet is obtained so that it can be used as a constraint formula.

The tablet can be divided into a rectangular prism and two halves of a round cylinder: figure 4 shows these divisions. For volume to be calculated, measurements of length, breadth, radius, and height are required. Therefore, its volume is given by the formula:

$$V = lbh + \pi r^2 h$$

The variable b, representing the diameter of the circle, can be replaced with $2r$:

$$V = 2rlh + \pi r^2 h$$

For this case, another constraint formula is required because both l and h need to be defined in terms of r and this is not possible with only the volume formula. As a result, the perimeter formula can be introduced. For the purpose of perimeter, the shape can be divided into a rectangle and two hemispheres. Hence, the formula is as follows:

$$P = 2l + 2\pi r$$

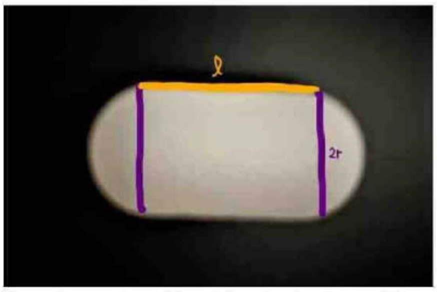

Figure 4: top view of the tablet taken by the candidate, edited using windows photos

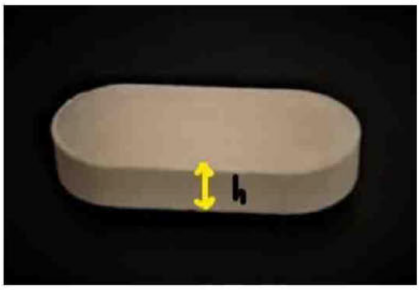

Figure 5: side view of the tablet taken by the candidate, edited using windows photos application

The tablet has a curved surface. Therefore, in order to obtain more accurate measurements, a thread was wrapped around the tablet (as shown in figure 5), then the length of the string was measured with a ruler.

Figure 6: view of the tablet taken by the candidate,

edited using windows photos

The measured values *are* $l = 1.10\ cm$, $b = 0.800\ cm$, $r = 0.400\ cm$ and $h = 0.300\ cm$.

These values are then substituted in the constraint volume formula:

$$V = 2(0.400)(1.10)(0.300) + \pi(0.400)^2(0.300) = 0.415\ cm^3$$

They are also substituted in the constraint perimeter formula:

$$P = 2(1.10) + 2\pi(0.400) = 4.71\ cm$$

The optimization is being done to find the minimum possible surface area. Therefore, let *SA* be surface area (cm^2), the objective function:

$$SA = 2lb + 2lh + \pi r^2 + \pi r^2 + \pi rh + \pi rh = 2lb + 2lh + 2\pi r^2 + 2\pi rh$$

Furthermore, *b* can be replaced with 2*r*:

$$SA = 4rl + 2lh + 2\pi r^2 + 2\pi rh$$

We could use the constraint volume formula to derive an expression for *h:*

$$0.415\ cm^3 = h\,(2lr + \pi r^2)$$

$$\frac{0.415}{(2lr + \pi r^2)} = h$$

This value can then be plugged into the *SA* formula as such:

$$SA = 4rl + 2l\left(\frac{0.415}{2lr + \pi r^2}\right) + 2\pi r^2 + 2\pi r\left(\frac{0.415}{2lr + \pi r^2}\right)$$

$$SA = 4rl + \frac{0.820l}{2lr+\pi r^2} + 2\pi r^2 + \frac{0.820\pi r}{2lr+\pi r^2}$$

We could use the constraint perimeter formula to derive an expression for 2*l* :

$$2l = P - 2\pi r$$

$$2l = 4.71 - 2\pi r$$

This value can then be plugged into the newly developed *SA* formula as such:

$$SA = 2r(4.71 - 2\pi r) + \frac{0.820(2.36 + \pi r)}{r(4.71 - 2\pi r) + \pi r^2} + 2\pi r^2 + \frac{0.820\pi r}{r(4.71 - 2\pi r) + \pi r^2}$$

$$SA = 9.43r - 2\pi r^2 + \frac{(1.96 + 0.820\pi r) + 0.820\pi r}{4.71r - 2\pi r^2}$$

$$SA = \frac{(4\pi^2 r^4 - 28.3\pi r^3 + 44.4r^2)}{4.71r - 2\pi r^2}$$

This equation can be simplified to $SA = \frac{(4\pi^2 r^3 - 28.3\pi r^2 + 44.4r)}{4.71 - 2\pi r}$ by factoring an r from both numerator and denominator.

Choosing the suitable optimization method based on continuity:

The simplified function of $SA = \frac{(4\pi^2 r^3 - 28.3\pi r^2 + 44.4r)}{4.71 - 2\pi r}$ has a vertical asymptote at r value of $\frac{4.71}{2\pi}$ cm. In other words, there is an essential discontinuity at this specific r value because there is a break in the function. Therefore, it can be said that the function is discontinuous at $r = \frac{4.71}{2\pi}$. This can be proved by using limits. Let the r value at which the continuity is being evaluated be a. If a function is continuous, $f(a)$ and $\lim_{r \to a} f(x)$ should both exist and be equal. Here, a is $\frac{4.71}{2\pi}$. In this case, neither of $f(\frac{4.71}{2\pi})$ and $\lim_{r \to \frac{4.71}{2\pi}} \left(\frac{(4\pi^2 r^4 - 28.3\pi r^3 + 44.4r)}{4.71 - 2\pi r}\right)$ exist and they are quite evidently not equal.

Furthermore, since the function is not continuous for $r \in IR$ and there are no closed intervals, the Extreme value theorem cannot be accepted for this case.

It is also possible to try the first derivative test using quotient rule:

Quotient rule: $\frac{(u'v - uv')}{v^2}$

Referring the quotient rule formula, u is $(4\pi^2 r^3 - 28.3\pi r^2 + 44.4r)$ and v is $4.71 - 2\pi r$. Furthermore, $u' = 12\pi^2 r^2 - 56.6\pi r + 44.4$ and $v' = 2\pi$

Now these values are substituted in the formula for quotient rule.

$$\frac{dSA}{dr} = \frac{(12\pi^2r^2 - 56.6\pi r + 44.4)(4.71 - 2\pi r) - (4\pi^2r^3 - 28.3\pi r^2 + 44.4r)2\pi}{(4.71 - 2\pi r)^2}$$

$$\frac{dSA}{dr} = \frac{-32\pi^3r^3 + 226\pi^2r^2 - 444\pi r + 209}{(4.71 - 2\pi r)^2}$$

$$\frac{dSA}{dr} = 0$$

$$\frac{-32\pi^3r^3 + 226\pi^2r^2 - 444\pi r + 209}{(4.71 - 2\pi r)^2} = 0$$

$$-32\pi^3r^3 + 226\pi^2r^2 - 444\pi r + 209 = 0$$

The zeros of this polynomial can be found using technology. The zeros can be detected by looking at the graph, as shown in figure 8 in the appendices.

It is also possible to calculate the remaining zeros by using one zero from the graph and employing the factor theorem.

The zeros can be reported aproximately as :

$r \approx 0.220$, $r \approx 0.750$, and $r \approx 1.280$

Additonally, I also came to the realization that it is possible to find the derivative of $SA = \frac{(4\pi^2r^3 - 28.3\pi r^2 + 44.4r)}{4.71 - 2\pi r}$ by directly employing polynomial divison in order to find the quotient and the remainder, the derivative of which can be found by simple differentiation. These findings are supported by Michael Weiss as such : “we can find the derivative of y = p(x) at a point using nothing more complicated than polynomial division and then computing q(a) = p′(a)” (Weiss).

Interval	**Testing in the function**
r <0.220 cm, let r = 0.100	$\frac{dSA}{dr}$ =$-32\pi^3(0.1)^3 + 226\pi^2(0.1)^2 - 444\pi(0.1) + 209 \approx$ 90.8 cm
0.220< r < *0.750* cm, let r = 0.500	$\frac{dSA}{dr}$ =$-32\pi^3(0.5)^3 + 226\pi^2(0.5)^2 - 444\pi(0.5) + 209 \approx$ -54.8
0.750 < r < *1.28* cm, Let r =1	$\frac{dSA}{dr}$ =$-32\pi^3(1)^3 + 226\pi^2(1)^2 - 444\pi(1) + 209 \approx 52.5$
r > 1.28 cm, let r = 3	$\frac{dSA}{dr}$ =$-32\pi^3(3)^3 + 226\pi^2(3)^2 - 444\pi(3) + 209 \approx$ -10690

Table 2: The values of r at specific intervals

As can be deduced from table 1, the graph is increasing at r <0.220, decreasing at *0.220*< r < *0.750*, increasing at *0.75 < r < 1.28 and decreasing for* r > 1.280. However, it is important to understand that the function has a break at $\frac{4.71}{2\pi}$ which approximately equals 0.750. One could assume that if there was not a break at this point, the correct value of the function local maximum could be found. At the same time, the other two zeros are relative minimums. Since we are looking for the lowest r value that can give the least surface area value, 0.220 cm can be accepted as the value that fulfils this objective.

The second derivative test could also be performed to ensure these results in the same way shown for round cylindrical tablet.

The graph of the surface area function which supports all the above statements is provided below in figure 7:

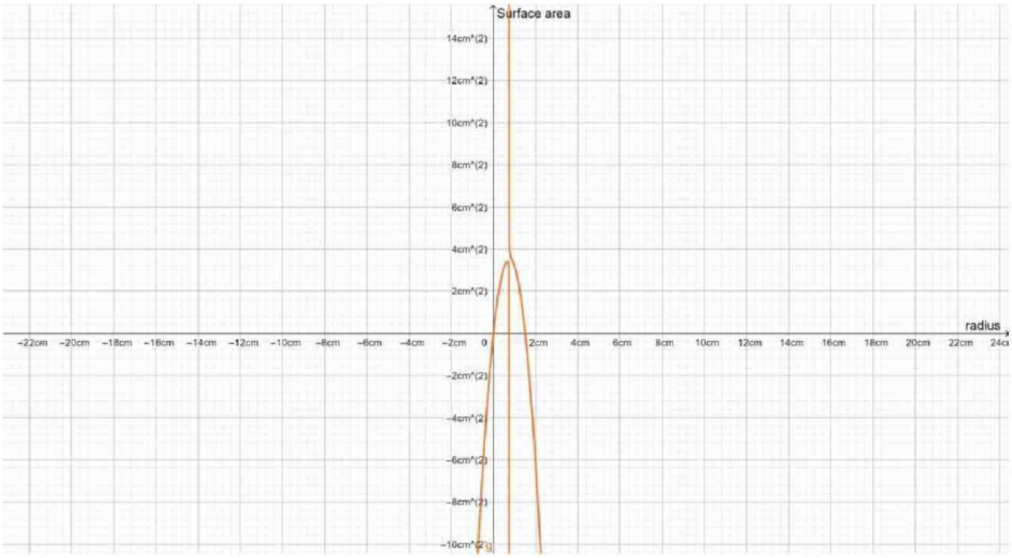

Figure 7: The graph of the function SA= $\frac{(4\pi^2 r^4 - 28.3\pi r^3 + 44.4r)}{4.71 - 2\pi r}$ – drawn by candidate using the GeoGebra Software

Having explored all the possible methods for the optimization of this shape, it is possible to reflect that the first derivative test along with sign diagram is the best method for this case because it can determine the relative minima, as well as the nature of the graph at certain r values: increasing or decreasing. It also gives insight about how the function would have behaved if there was not a break in it.

Finding all optimized dimensions:

The minimum r value can now be used for deriving the other dimensions:

1) $2l = 4.71 - 2\pi r$

$2l = 4.71 - 2\pi(0.22) \approx 3.33\ cm$

$l \approx 1.67$

2) $\frac{0.415}{(2lr+\pi r^2)} = h$

$h \approx 0.790$

Conclusion

The aim of this exploration was to find the optimized dimensions of the two different shapes of 500 mg paracetamol tablet. The optimized dimensions for the round cylindrical tablet was obtained to be 0.600 cm for radius and 2 cm for height. These values are different from the original values which were 1.20 cm for radius and 0.300 cm for height. It appears that the radius has been decreased and height has been increased. As for the case of the capsular tablet, the obtained radius measures 0.200 cm, the length measures 1.67 cm, and the height measures 0.790 cm. The original values were 0.400 cm, 0.300 cm, and 1.10 cm for radius, height, and length respectively. The radius is decreased, but both length and height are increased for the lowest optimum surface area.

Both these optimized dimensions suggest that tablets should be thinner but more elongated, which cannot be effectively applicable to the tablet production. This is because, such a shape reduces the compactness of the tablet and makes it more susceptible to breaking apart at an undesirable location in the body. Eventhough the consumer's comfort in swallowing the tablet is important, it is more important that the need for the medicine contained in the tablet is completely fulfilled.

In addition, there were certain limitations involved in this exploration, one being the numerous steps involved in calculating derivatives. There were multiple steps involved and many values were rounded in different places. This could be the reason why the zeros obtained are slightly different from the values obtained using technology. Another limitation was that the tablets were small, as a result, measuring them was associated with certain degree of uncertainty attributed to the ruler and to the human eye.

On the other hand, this exploration had many strengths. It involved an analysis of the various optimization methods and which one is best suited for each function. This exploration also allowed me to use my knowledge of different areas of mathematics to solve one problem and provided an experience of applying mathematics to a real-life problem in society.

Bibliography

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Appendices

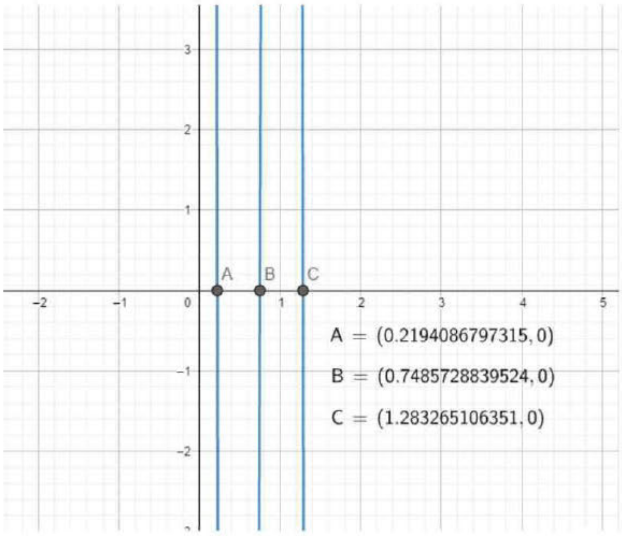

Figure 8: the function for the first derivative of SA: $-32\pi^3r^3 + 226\pi^2r^2 - 444\pi r + 209$, with A,B, and C showing the coordinates foe the zeros of the function—drawn by candidate using GeoGebra software