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Application of Simpson´s and trapezoidal formulas for volume calculation of subsurface structures - recommendations

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Abstract

In nature, most of the subsurface geological structures have an asymmetric shape. To estimate the volume of such structures numerical integration is used. Two methods have been analysed for volume estimation of geological structures: trapezoidal and Simpson´s method. Both methods estimate the volume of the structure, because they have a certain error in the calculation. Two examples of the hypothetical hydrocarbon reservoirs are presented: massive and layered ones. Differences between volume calculations obtained by trapezoidal and Simpson formulas mostly are not significant. Larger number of sections generally leads to smaller differences between volumes calculated by trapezoidal and Simpson rules. In even number of sections, the recommendation is to apply Simpson and top formulas. If number of sections is odd, the combination of Simpson's formula for $\boldsymbol{n-1}$ sections, trapezoidal for $\boldsymbol{n}$-*th* section and top formulas for the rest is appropriate.

Keywords: anticline, numerical integration, trapezoidal rule, Simpson´s rule

1. Introduction

Knowing the approximate volume of the structures is necessary for, e.g., economic analysis, prediction of migration, geological evolution etc. After geological, geophysical and geochemical research and drilling explorations such volume calculation can be performed. Such analysis is also often part of stratigraphy, reservoir, petrophysical or similar modelling. Volume calculation is in most cases part of hydrocarbon reserves estimation, and is largely dependent on size and reliability of input dataset(s). We present reservoir volume calculation by applying two rules: trapezoidal and Simpson´s ones. Their results are compared and recommendation of application, based on the number of isopaches, is given.

2. Basics about numerical integration

Geological structures such as anticlines are the most common hydrocarbon traps (e.g., **Malvić & Velić, 2008**). However, such structures mostly have partially irregular shape and geometrical approximation with truncated cone is not ideal (e.g., **Malvić et al., 2014**). For this reason analytical integration cannot be applied to estimate volume of such structures. However, if the area $A(x)$ of cross section parallel to the plane yz (**Fig. 1**) is known, integral formulation (**Eq. 1)** can be used to compute the volume of a body in certain boundaries - a, b.

$$V = \int_a^b A(x)dx \qquad \text{Eq. 1}$$

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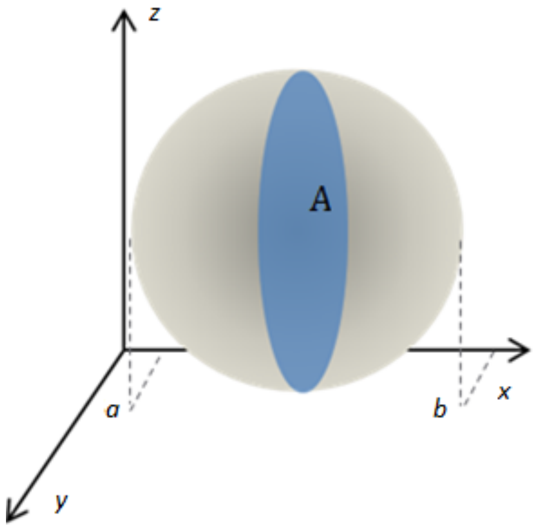

Figure 1: A solid object with boundaries extending from $x = a$ to $x = b$

In this way the volume of irregular body cannot be exactly calculated. Consequently, approximate methods for the volume calculation are used like trapezoidal and Simpson´s method (e.g., **Scitovski, 2014**).

2.1. Trapezoidal rule

Trapezoidal rule is based on the method in which curve f is approximated with straight line L, as shown on **Fig. 2**. The area bounded by the curve f, lines $x = a$ and $x = b$, and the axis x is approximated by the area of the trapezoid with the bases of lengths $f(a)$ and $f(b)$, and the height $(b - a)$ (e.g., **Čančarević, 2016**). Equation of the line L passes through the points $A(a, f(a))$ and $B(b, f(b))$ is (**Eq. 2**)

$$L(x) = \frac{f(b)-f(a)}{b-a}(x - a) + f(a). \qquad \text{Eq. 2}$$

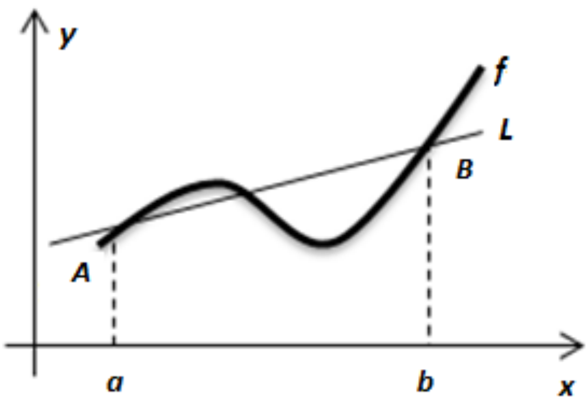

Figure 2: Approximation of the curve f with straight line L

The area of the trapezoid is obtained by integrating function L (**Eq. 3**) on the segment $[a, b]$, so we have (**Eq. 3**):

$$\int_a^b f(x)dx \approx \int_a^b L(x)dx = \frac{b-a}{2}\left(f(a) + f(b)\right). \qquad \text{Eq. 3}$$

With this method approximation is relatively good, but there are still possible errors. So, to minimize the error it is necessary to divide interval $[a, b]$ with points $a = x_0, x_1, x_2, \ldots, x_{n-1}, x_n = b$ on n equally long segments, **Figure 3**.

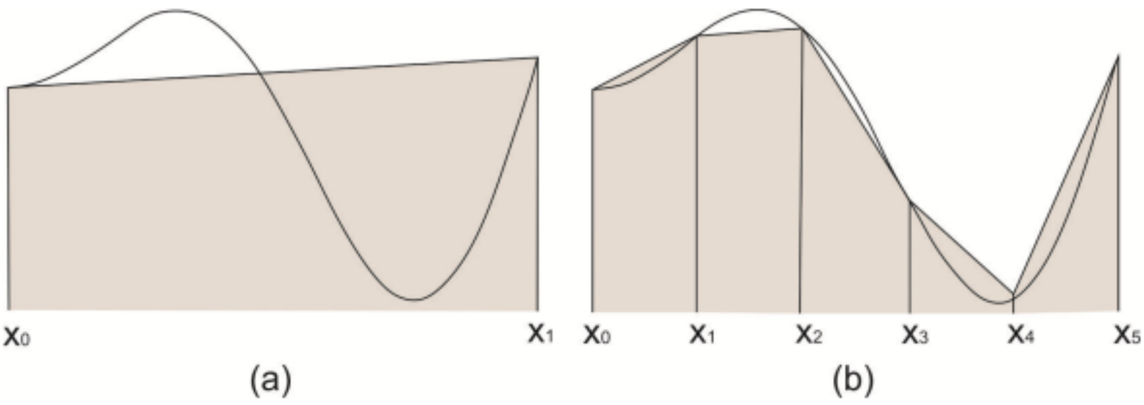

Figure 3: Trapezoidal rule with one interval (a) and five subintervals (b)

Final form of the trapezoidal rule is **(Eq. 4)**:

$$\int_a^b f(x)dx \approx \frac{h}{2}\left(y_0 + y_n + 2(y_1 + y_2 + \cdots + y_{n-1})\right) \quad \text{Eq. 4}$$

where are:

$y_0 = f(x_0), y_1 = f(x_1), \dots, y_{n-1} = f(x_{n-1}), y_n = f(x_n)$;

$h = \frac{b-a}{n}$ - *length of each subinterval.*

With more subintervals the error is smaller, but still present. To calculate the error obtained with trapezoidal rule, the second derivation of function f is required, (**Eq. 5**):

$$\varepsilon \leq \frac{(b-a)h^2}{12} M \quad \text{Eq. 5}$$

where are:

ε - *error*;

$M = \max_{x \in [a,b]} |f''(x)|$;

$h = \frac{b-a}{n}$ - *length of each subinterval.*

If *f* is a first degree polynomial, respectively function whose graph is a straight line, solution error is zero.

2.1. Simpson´s rule

Simpson´s rule is based on the idea to approximate the curve f with a second-degree polynomial (**Eq. 6**):

$$P(x) = a_0 x^2 + a_1 x + a_2. \quad \text{Eq. 6}$$

Graph of the function P is a parabola (see **Fig. 4**), where unknown coefficients a_0, a_1, a_2 are calculated from **Eq. 7**:

$$P(a) = f(a),\ P\left(\frac{a+b}{2}\right) = f\left(\frac{a+b}{2}\right), P(b) = f(b). \quad \text{Eq. 7}$$

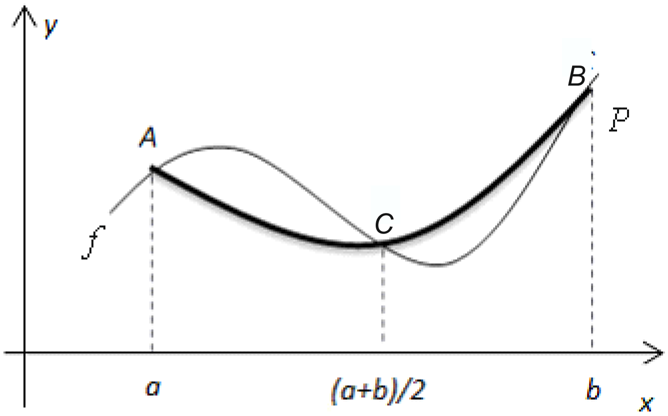

Figure 4: Interpolation of the curve f with P

Then, integration of function P on segment $[a,b]$ is performed, **Eqs. 8** and **9:**

$$\int_a^b P(x)dx = \int_a^b (a_0x^2 + a_1x + a_2)dx = \frac{1}{6}(b-a)\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right); \quad \text{Eq. 8}$$

$$\int_a^b f(x)dx \approx \int_a^b P(x)dx = \frac{1}{6}(b-a)\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right). \quad \text{Eq. 9}$$

Like in the trapezoidal rule, for more precise result it is required to divide interval $[a,b]$ into smaller equidistant intervals. Interval $[a,b]$ is divided with points $a = x_0, x_1, x_2, \dots, x_{n-1}, x_n = b$ on even number $n = 2m$ subintervals of the same length $h = \frac{b-a}{n}$, **Figure 5**.

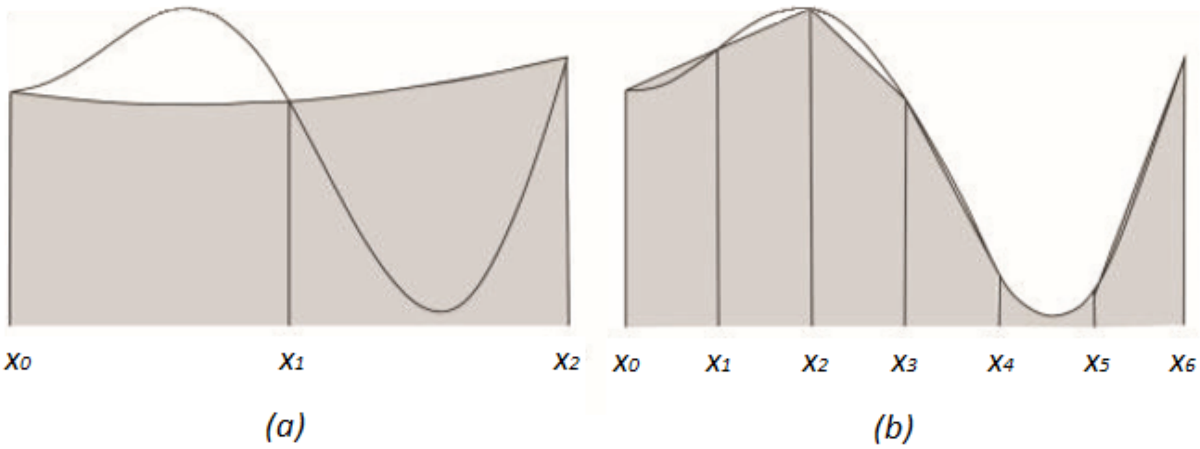

Figure 5: Simpson's rule with two subintervals (a) and with $2m = 6$ subintervals (b)

The equation **Eq. 9** is used on the segments $[x_0, x_2], [x_2, x_4], \dots, [x_{n-4}, x_{n-2}], [x_{n-2}, x_n]$ (each segment consists of two subintervals). After summing up the results, general form of Simpson´s rule is obtained (**Eq. 10**):

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(y_0 + y_n + 4(y_1 + y_3 + \dots + y_{n-1}) + 2(y_2 + y_4 + \dots + y_{n-2})\right) \quad \text{Eq. 10}$$

where are:

$y_0 = f(x_0), y_1 = f(x_1), \dots, y_{n-1} = f(x_{n-1}), y_n = f(x_n);$

$h = \frac{b-a}{n}$ – *length of each subinterval.*

Although this method is more precise then trapezoidal method, error exists due to approximation. It can be calculated with **Eq. 11**:

$$\varepsilon \le \frac{(b-a)h^4}{180} M; \qquad \text{Eq. 11}$$

where are:

ε – *error*;

$M = \max_{x\in[a,b]} |f^{iv}(x)|$;

$h = \frac{b-a}{n}$ - *length of each subinterval* (*further in the text is marked with „e“*).

Observe that in the case when f is a polynomial whose degree is at most three, the result is precise, i.e. error is zero.

3. The application of numerical integration in the description of the hydrocarbon reservoir

Numerical integration is used in calculating the approximate volume of hydrocarbons reservoirs. Geology problems of this type have been studied earlier (e.g., **Malvić et al., 2014**). With the aim of economic benefit, it is necessary to get enough data for mapping and volume calculations, with minor or no additional need to collect new data. Moreover, hydrocarbon reservoirs are most commonly closed with structural traps, i.e. anticlines. Such examples (e.g., **Malvić and Velić, 2008; Velić, 2007; Velić et al., 2015)**, based on this structure, are used in this analysis (**Figs. 6** and **7**).

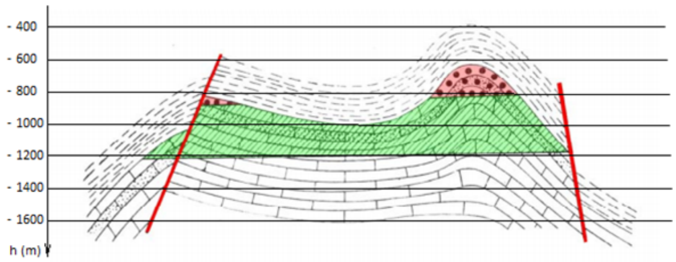

Figure 6: Massive type of the hydrocarbons reservoir

Massive type of reservoir (**Fig. 6**) is hydrocarbon accumulation in the “massive” rock section (usually several lithotypes) with known and well reservoir properties. Similarly, but not the same, “layered” reservoir (**Fig. 7**) is trapped into one strata or depositional unit, bordered with known bottom and roof (isolator) beds. Such reservoir usually has better (isotropic on smaller scale) petrophysical properties than the massive one.

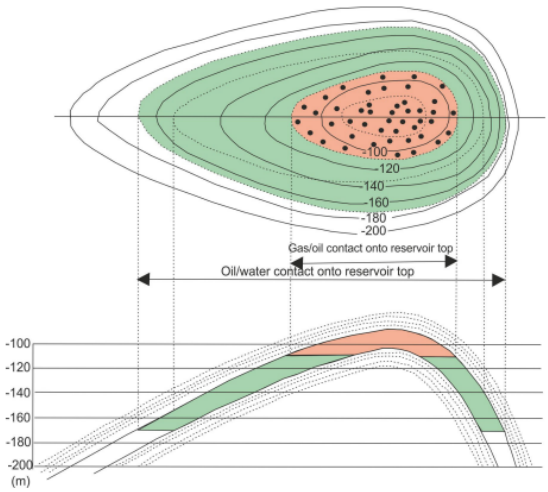

Figure 7: “Layered” reservoir as irregular brachianticline

3.1. Volume calculation in massive reservoir

Isopach (contour) map for the top of massive reservoir is shown at **Fig. 8**. The contact is above the basement, so the volume is calculated between such contact and the top map. Brachianticline is shown using equidistance of 5 m, and structure dips are less than 20°.

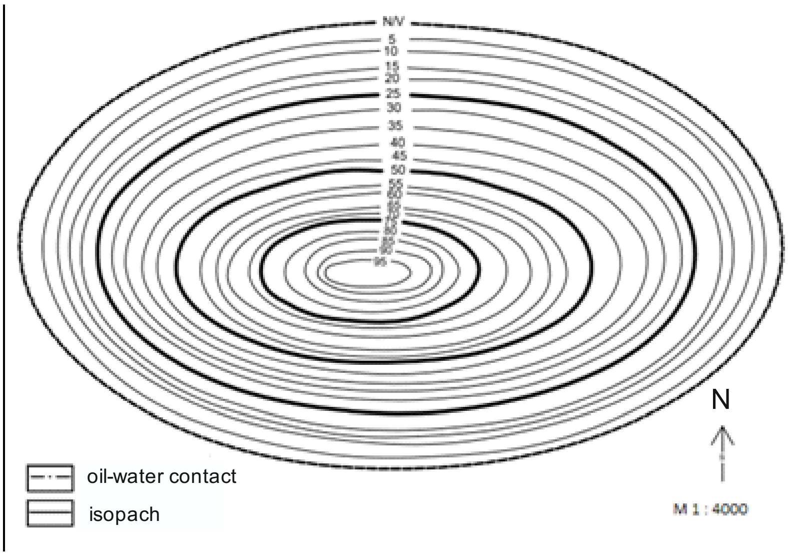

Figure 8: *Isopach map of massive type reservoir. Volume between contact water/hydrocarbons – reservoir top. Top height is 1 m.*

So, the structure has been cut with isopach planes, every 5 m (equidistance). Section areas are measured by planimeter, instrument used for measuring the area of irregular surfaces (e.g., **Malvić, 2015**). Absolute difference between starting and ending point observed on planimeter during measuring of isopach is multiplied by a multiplying constant (which depends on scale). The result is area bounded with observed isopach in squared meters. Here the scale 1:4000 has been multiplied with constant of 1600. The areas a_i are shown in **Table 1.**

Isopach no.	1st starting point of planimeter	2nd finishing point of planimeter	|1st – 2nd|	Absolute area a_i [m²]
0	4202	6372	2170	3 472 000
1	6434	8405	1971	3 153 600
2	1094	2891	1797	2 875 200
3	2939	4559	1620	2 592 000
4	1619	3086	1467	2 347 200
5	4675	5982	1307	2 091 200
6	4450	5620	1170	1 872 000
7	5710	6730	1020	1 632 000
8	6759	7646	887	1 419 200
9	7768	8522	754	1 206 400
10	8593	9233	640	1 024 000
11	9325	9842	517	827 200

12	37	467	430	688 000
13	566	890	324	518 400
14	1025	1273	248	396 800
15	1374	1544	170	272 000
16	1651	1755	104	166 400
17	1848	1906	58	92 800
18	1955	1987	32	51 200
19	2046	2058	12	19 200
20	2106	2109	3	4800

Table 1: Planimeter results for section crossing massive reservoir (contact-top)

3.1.1. Case 1: massive reservoir divided with even number of sections

First case included even number of section, i.e. odd number of isopach. Results obtained with Simpson´s formula are shown in **Table 2**. The preciseness has been simulated with different equidistance - 5, 10, 25 and 50 m. Moreover, the total volume of reservoir is always increased with small additional volume above the last isopach, named as "top". This volume is defined by height smaller than equidistance. The volume V_T of the top (**Eq. 14**) is calculated as an arithmetic average of the results of the following two formulas, i.e. pyramidal (**Eq. 12**) and spherical approximation (**Eq. 13**), given, e.g., in **Korać (2015)**:

$$V_p = \frac{h_n\, a_n}{3}, \qquad \text{Eq. 12}$$

where are:

V_p - *pyramidal approximation;*
h_n - *distance from the last isopach to the top of the structure;*
a_n - *area bounded with the last isopach;*

$$V_{sf} = \frac{h_n^3 \Pi}{6} + \frac{a_n\, h_n}{2}, \qquad \text{Eq. 13}$$

where are:

V_{sf} - *spherical approximation;*
h_n - *distance from the last isopach to the top of the structure;*
a_n - *area bounded with the last isopach;*

$$V_T = \frac{1}{2}\left(V_p + V_{sf}\right). \qquad \text{Eq. 14}$$

By summing a volume V_S calculated with Simpson´s formula (even sections) plus a volume V_T of the top structure, the total volumes are given in **Table 2**.

e (m)	Number of sections	Used areas	Volumes calculated with Simpson's and top formulas $V_S + V_T$ (m³)
5	20	$a_0, a_1, \dots, a_{19}, a_{20}$	124 628 667
10	10	$a_0, a_2, \dots, a_{18}, a_{20}$	125 319 334
25	4	$a_0, a_5, a_{10}, a_{15}, a_{20}$	124 815 334
50	2	a_0, a_{10}, a_{20}	126 215 334

Table 2: Volume (**Figure 8**) calculated with Simpson's and top formulas for even number of sections

That was continued with calculation of the total volumes by replacing Simpson's with trapezoidal formula, that is, the total volumes are obtained by summing volumes V_t calculated with a trapezoidal formula and the volume V_T of the top. The results are given in **Table 3**.

e (m)	Number of sections	Used areas	Volumes calculated with trapezoidal and top formulas $V_t + V_T$ (m^3)
5	20	$a_0, a_1, \dots, a_{19}, a_{20}$	124 918 000
10	10	$a_0, a_2, \dots, a_{18}, a_{20}$	125 786 000
25	4	$a_0, a_5, a_{10}, a_{15}, a_{20}$	128 142 000
50	2	a_0, a_{10}, a_{20}	138 122 000

Table 3: Volume (**Figure 8**) calculated with trapezoidal and top formulas for even number of sections

To estimate the error, a deviation $\frac{|V_t - V_S|}{\min\{V_t, V_S\}}$ is calculated and the results are shown in percentage (**Table 4**). As can be seen, the deviation is nowhere larger than 20 %, what is considered as a limit to accept calculation with Simpson's formula as valid for structure volume (e.g., in **Malvić et al., 2104**; **Malvić, 2015**).

e (m)	Volumes calculated with Simpson's and top formulas $V_S + V_T$ (m^3)	Volumes calculated with trapezoidal and top formulas $V_t + V_T$ (m^3)	$\Delta V = \lvert V_t - V_S \rvert$ (m^3)	Deviations $\frac{\Delta V}{\min\{V_t, V_S\}}$ (%)
5	124 628 667	124 918 000	289 333	0.23
10	125 319 334	125 786 000	466 666	0.37
25	124 815 334	128 142 000	3 326 666	2.67
50	126 215 334	138 122 000	11 906 666	9.43

Table 4: Simpson's and trapezoidal (plus top) volumes of structure (**Figure 8**), and their deviations – even number of sections

3.1.2. Case 2: massive reservoir divided with odd number of sections

That case included odd number of sections, i.e. even number of isopach. However, Simpson's formula is designed only for even number of sections. So, the Simpson's rule was applied for the volume up to penultimate isopach, i.e. for $n-1$ sections. Consequently, for the space between penultimate and last isopaches, trapezoidal rule has been used. At the end, the volume V_T of the "top" is added.

So, the total volume is a summation of $V_S^{(1,\dots,n-1)}$ (volume obtained by Simpson's formula for first $n-1$ sections), $V_t^{(n)}$ (volume obtained by a trapezoidal formula for n-th section) and V_T (volume of the top). In **Table 5** is given a calculation for massive reservoir divided with odd number of sections. Differences between mixed and pure trapezoidal approach are shown in **Table 6**.

e (m)	Number of sections	Used areas	$V_S^{(1,\dots,n-1)}$ (m^3)	$V_t^{(n)}$ (m^3)	$V_S^{(1,\dots,n-1)} + V_t^{(n)}$ (m^3)	$V_S^{(1,\dots,n-1)} + V_t^{(n)} + V_T$ (m^3)
20	5	$a_0, a_4, a_8, a_{12}, a_{16}, a_{20}$	124 117 333	1 712 000	125 829 333	125 831 333

Table 5: Volume (**Figure 8**) calculated with Simpson's (n − 1 sections), trapezoidal (n-th section) and top (above n-th section) formulas – odd number of sections

e (m)	Number of sections	Volume calculated with Simpson's (first $n-1$ sections), trapezoidal (n-th section) and top (above n-th section) formulas $V_S^{(1,\ldots,n-1)} + V_t^{(n)} + V_T$ (m³)	Volume calculated with trapezoidal (n sections) and top (above n-th section) formulas $V_t^{(1,\ldots,n)} + V_T$ (m³)	$\Delta V = \lvert V_t^{(1,\ldots,n-1)} - V_S^{(1,\ldots,n-1)} \rvert$ (m³)	Deviation $\frac{\Delta V}{\min\{V_t^{(1,\ldots,n-1)}, V_S^{(1,\ldots,n-1)}\} + V_t^{(n)}}$ (%)
20	5	125 831 333	127 186 000	1 354 667	1.08

Table 6: Simpson's and trapezoidal total volumes of reservoir, and their difference and deviation – odd number of sections

3.2. Volume calculation in layered reservoir

In this case, layered reservoir with anticline trap is presented. However, the water-hydrocarbons contact cut both, reservoir top and bottom. So, the reservoir volume is a simple difference between volumes of contact-reservoir top and contact-reservoir bottom. Valid isopach map for volume contact-reservoir top is given previously at **Fig. 8**. However, the isopach map for volume contact-reservoir bottom is given at **Fig. 9**. Planimeter results for the isopachs on **Figure 9** are given in **Table 7**. For the isopach maps contact-top the values in **Tables 1-3** are valid also here.

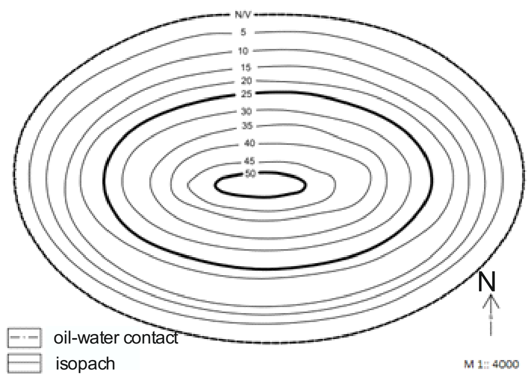

Figure 9: *Isopach map of layered type reservoir. Volume between contact water/hydrocarbons – reservoir bottom. Top height is 1 m.*

Isopach no.	1st starting point of planimeter	2nd finishing point of planimeter	|1st – 2nd|	Absolute area a_i [m²]
0	1164	2010	846	1 353 600
1	2114	2754	640	1 024 000
2	2825	3332	507	811 200
3	3433	3820	387	619 200
4	3892	4185	293	468 800
5	4280	4482	202	323 200
6	4539	4670	131	209 600
7	4747	4835	88	140 800
8	4914	4962	48	76 800
9	5040	5061	21	33 600
10	5103	5105	2	3 200

Table 7: Planimeter results for section crossing layered reservoir (contact-bottom)

3.2.1. Case 1: layered reservoir divided with even number of sections

Here is used equidistance of 5 and 25 m. The results are compared for volume of n sections (even number) both for Simpson's and trapezoidal formulas, absolute differences and deviations (**Table 8**).

e (m)	Number of sections	Used areas	Volumes calculated with Simpson's and top formulas $V_S + V_T$ (m³)	Volumes calculated with trapezoidal and top formulas $V_t + V_T$ (m³)	$\Delta V = \lvert V_t - V_S \rvert$ (m³)	Deviations $\frac{\Delta V}{\min\{V_t, V_S\}}$ (%)
5	10	$a_0, a_1, \dots, a_9, a_{10}$	21 756 000	21 929 334	173 334	0.80
25	2	a_0, a_5, a_{10}	22 081 334	25 041 334	2 960 000	13.40

Table 8: Volume (**Figure 9**) calculated with Simpson's and trapezoidal formulas – n (even) sections (contact-bottom)

The error is, in all cases, less than 20% what means that Simpson's formula for n sections and selected equidistance can be used properly. Eventually, it was possible to calculate total volume of layered reservoir as the difference between contact/top and contact/bottom. The results are given in **Table 9**.

e (m)	Layered reservoir, total volume (top-bottom, m³)
5	102 872 666
25	102 734 000

Table 9: Total volume of layered bed in m³ – even number of sections

3.2.2. Case 2: layered reservoir divided with odd number of sections

Layered reservoir has also been divided with odd number of sections. It meant that mutually was applied Simpson's formula (for even number of sections, i.e. first $n-1$ sections), trapezoidal formula for the last (n^{th}) section and top formulas (above the n^{th} section), as shown in **Table 10**. For comparison, in **Table 11** are given results if only trapezoidal formula was applied for n sections.

e (m)	Number of sections	Used areas	$V_S^{(1,\dots,n-1)}$ (m³)	$V_t^{(n)}$ (m³)	$V_S^{(1,\dots,n-1)} + V_t^{(n)} + V_T$ (m³)
10	5	$a_0, a_2, a_4, a_6, a_8, a_{10}$	21 504 000	400 000	21 905 334

Table 10: Volume (**Figure 9**) calculated with Simpson's, trapezoidal and top formulas – odd number of sections (contact-bottom)

e (m)	Number of sections	Used areas	$V_t^{(1,\dots,n)} + V_T$ (m³)
10	5	$a_0, a_2, a_4, a_6, a_8, a_{10}$	22 449 334

Table 11: Volume (**Figure 9**) calculated with trapezoidal formula - odd number of sections (contact-bottom)

Those two approaches yielded slightly different results, which are compared in **Table 12** for equidistance of 10 m. Differences were much less than 20 %, so mutual Simpson's and trapezoidal approach was valid for using.

Volume calculated with Simpson's (first n−1 sections), trapezoidal (n-th section) and top (above n-th section) formulas $V_S^{(1,\dots,n-1)} + V_t^{(n)} + V_T$ (m³)	Volume calculated with trapezoidal (n sections) and top (above n-th section) formulas $V_t^{(1,\dots,n)} + V_T$ (m³)	$\Delta V = \lvert V_t^{(1,\dots,n-1)} - V_S^{(1,\dots,n-1)} \rvert$ (m³)	Deviation $\frac{\Delta V}{\min\{V_t^{(1,\dots,n-1)}, V_S^{(1,\dots,n-1)}\} + V_t^{(n)}}$ (%)
21 905 334	22 449 334	544 000	2.48

Table 12: Simpson's and trapezoidal total volumes of reservoir, and their difference and deviation – odd number of sections (contact-bottom)

Now, it was possible to calculate the total volume of layered reservoir as a difference between volumes contact/top – contact/bottom (**Table 13**).

e (m)	Layered reservoir, total volume (top-bottom, m³)
10	103 414 000

Table 13: Total volume of layered reservoir – odd number of sections

5. Conclusions

The understanding of calculation procedure is more important than data quantity. Presented results proved that statement. It is also necessary to understand mathematical backgrounds of given approaches as a base for regular and correct calculations of subsurface structure's volumes. Here are the main recommendations and conclusions derived from presented methods and results:

1. Simpsons's rule is more accurate because it depends on h^4 and error will reach zero faster unlike trapezoidal rule where error depends on h^2. For Simpson's rule, error is zero when f is a polynomial whose degree is at most three, while for a trapezoidal rule error is zero when f is a polynomial of the first degree.
2. Method of calculation depends on the number (more is better) of sections (e.g., **Table 9**), and more – whether such number is even or odd.
3. The new approach is proposed for odd number of sections. Simpson's formula is used till penultimate isopach (even number of parts), and volume of the last section is calculated using the trapezoidal rule. The result is a sum of those two volumes.
4. All volumes need to be increased with a volume of the top, i.e. volume above the last isopach.
5. Different calculations, for the same number of sections, can be relatively compared using the deviation formula.
6. Described approach is valid for using in the case of "symmetrical" structures like anticlines or gently elongated brachianticlines.

6. References

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Abstract in Croatian

Preporuke za uporabu Simpsonove i trapezne formule kod izračuna volumena dubinskih struktura

Procjenu volumena geoloških struktura možemo izračunati integriranjem. Kako dubinske strukture najčešće nisu pravilnih oblika ne može se primijeniti analitičko integriranje već se koristi numeričko integriranje, tj. trapezna i Simpsonova formula. Oba pristupa približno određuju volumen ležišta. Ovdje su opisana dva primjera dubinskih struktura, ujedno i ležišta ugljikovodika. To su masivno i slojno ležište. Razlike između volumena dobivenih trapeznom i Simpsonovom formulom uglavnom nisu velike. Veći broj odsječaka u pravilu vodi do manjeg odstupanja između rješenja dobivenih trapeznim i Simpsonovim pravilom. Kod parnoga broja odsječaka preporučena je uporaba Simpsonove formule te one za kapu. Kod njihova neparnoga broja predložen je izračun prema Simpsonovoj formuli za dio volumena koji uključuje *n-1* odsječaka, zatim prema trapeznoj za *n*-ti odsječak, te prema formulama za volumen kape za ostatak iznad toga odsječka.

Ključne riječi: antiklinala, numerička integracija, trapezno pravilo, Simpsonovo pravilo

Authors contribution

Josipa Pavičić (undergraduate student) finished this topic as her bachelor thesis, interpolated maps, using planimeter and make calculations. **Željko Andreić** (Full Professor) supervised mathematical equations and style. **Tomislav Malvić** (Full Professor) and **Josipa Velić** (Prof. Emerita) supervised the geological interpolation, planimeter results and reservoir geology theory. **Rajna Rajić** (Full Professor) supervised mathematical consistency of mathematical part, especially numerical integration formulas.