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Volume calculation of subsurface structures and traps in hydrocarbon exploration – a comparison between numerical integration and cell based models

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Abstract: The volume calculation of geological structures is one of the primary goals of interest when dealing with exploration or production of oil and gas in general. Most of those calculations are done using advanced software packages but still the mathematical workflow (equations) has to be used and understood for the initial volume calculation process. In this paper a comparison is given between bulk volume calculations of geological structures using trapezoidal and Simpson's rule and the ones obtained from cell-based models. Comparison in calculation is illustrated with four models; dome – 1/2 of ball/sphere, elongated anticline, stratigraphic trap due to lateral facies change and faulted anticline trap. Results show that Simpson's and trapezoidal rules give a very accurate volume calculation even with a few inputs (isopach areas – ordinates). A test of cell based model volume calculation precision against grid resolution is presented for various cases. For high accuracy, less the 1% of an error from coarsening, a cell area has to be 0.0008% of the reservoir area.

Keywords: cell-based volume; Simpson's rule; trapezoidal rule; volume calculation; hydrocarbons

1 Introduction

Estimation of areas and volumes is one of the most basic engineering tasks in hydrocarbon exploration and pro-

duction [1]. Today, volume estimation of subsurface structures, *i.e.* hydrocarbon reservoir volume calculation, is usually done using various modelling software. For proper application and result interpretation it is necessary to understand how the software computes and handles inputs. Part of computer algorithm is based on mathematical equations that approximate volume and part on division of volume in extremely large number of cells and their summation. The exact process behind the computer algorithm is a part of a trade secret and will not be discussed within this manuscript.

In this context, the comparison between these two approaches is very useful for understanding proper choice and use of any of them. It is why hydrocarbon reservoir volume calculation with Simpson's and trapezoidal rules and the ones obtained from cell based model with Schlumberger Petrel software is given. The differences in the calculated volumes are analyzed between software based approach and mathematical approximation methods. Level of the detail needed for an accurate volume calculation when using software solutions is also addressed here. In other words, which level of resolution of model grid (cell size) is good enough for accurate volume calculation but not too detailed for other modelling processes (porosity distribution, etc.). Only the horizontal projection dimensions of a cell are regarded in this case. For this purpose Schlumberger Petrel modeling software will be used for the cell based volume calculation. It should be noted that only bulk volume calculation was performed. Cases presented correspond mainly to conventional hydrocarbon accumulations – oil or gas in sandstones like the ones described in [2–4] but can also be applied when unconventional reservoirs [5, 6] volume is calculated.

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2 Short theoretical review of some of the volume calculation methods

A short overview of the theoretical backgrounds of methods used for volume calculation is presented. These included numerical integration processes (Trapezoidal and Simpson's rule) and cell based model approach.

The first two approaches are by approximation methods of definite integrals which may be determined using numerical integration. Even when dealing with advanced methods of integration there are many mathematical functions which cannot be integrated analytically, thus approximation has to be used [7]. More precisely, determining the value of a definite integral is in fact finding the area between the horizontal axis and specified ordinates, *i.e.* between a curve. These ordinates in hydrocarbon volume calculation refer to the area bound by isopachs contours in a reservoir thickness maps.

2.1 The trapezoidal rule

Trapezoidal rule is a fairly simple mathematical approach described in [8, 9]. It relates to a definite integral denoted by $\int_a^b f(x) dx$. If f is positive, then the integral represents the area bounded by the curve $y = f(x)$ and the lines $x = a$; $x = b$ and $y = 0$: (Figure 1).

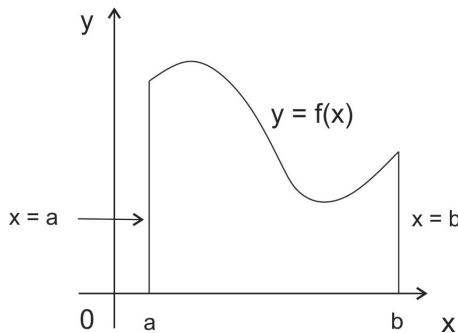


Figure 1: Example of area bounded by graph $y = f(x)$ and limits $x = a$, $x = b$ and $y = 0$.

If the interval of integration was divided into n equal intervals each of width d , such that $d = \frac{b-a}{n}$ where $a = x_0 < x_1 < \dots < x_{n-1} < x_n = b$ then the trapezoidal approximation was applied by joining the tops of the ordinates by

straight lines, and the outcome is

$$\int_a^b f(x) dx = \sum_{i=1}^n \int_{x_{i-1}}^{x_i} f(x) dx$$

$$\approx \frac{1}{2} \sum_{i=1}^n (x_i - x_{i-1}) (f(x_{i-1}) + f(x_i))$$

i.e.

$$I = \int_a^b f(x) dx \approx I_{trap.} = \frac{d}{2} \left[f(a) + f(b) + 2 \sum_{i=1}^{n-1} f(x_i) \right] \quad (1)$$

2.2 The Simpson's rule

The core of the delineation in trapezoidal approximation is founded in joining the top of two successive ordinates by a straight line, *i.e.* by usage of a polynomial of degree 1 ($y = a + bx$) [8, 9]. With Simpson's rule the approximation is done by joining the tops of three successive ordinates by a parabola, *i.e.* by a polynomial of degree 2 ($y = a + bx + cx^2$) [8, 9]. Therefore, a more precise approximation was obtained with Simpson's rule than with the trapezoidal rule. If parabola passes through the points $(a, f(a))$, $(b, f(b))$, $(c, f(c))$, where $c = \frac{1}{2}(a + b)$ then

$$\int_a^b f(x) dx \approx \frac{1}{6} (b - a) \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]. \quad (2)$$

In practice, interval $[a, b]$ is divided into $2n$ subintervals $a = x_0 < x_1 < \dots < x_{2n-1} < x_{2n} = b$ of the same length $h = \frac{b-a}{2n}$. If Simpson's rule is applied on the successive pair of interval $[x_{2i-2}, x_{2i}]$ where $i = 1, \dots, n$ then

$$\int_{x_{2i-2}}^{x_{2i}} f(x) dx \approx \frac{1}{6} (x_{2i} - x_{2i-2}) [f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})],$$

whereas

$$\int_a^b f(x) dx = \sum_{i=1}^n \int_{x_{2i-2}}^{x_{2i}} f(x) dx \approx \frac{1}{6} \sum_{i=1}^n (x_{2i} - x_{2i-2}) [f(x_{2i-2}) + 4f(x_{2i-1}) + f(x_{2i})]$$

and finally,

$$I = \int_a^b f(x) dx \approx I_{Simps.} \quad (3)$$

$$= \frac{h}{3} \left[f(a) + f(b) + 2 \sum_{i=1}^{n-1} f(x_{2i}) + 4 \sum_{i=1}^n f(x_{2i-1}) \right].$$

It is important to emphasize that Simpson's rule can only be applied when an even number of intervals is chosen, namely, an odd number of ordinates [8–10].

2.3 Cell based volume calculation

Cell based models are parts of the subsurface made of large number of cells (pillars). A cell size is defined by the grid resolution of the model which is user defined. These grids can be structured or unstructured [11]. Structured grids are commonly used in petroleum geological purposes. When regarding vertical resolution of a model, in a simple case these are restructured top and bottom surfaces. Grid geometry in a non-faulted model is simple but errors on structure margins could be compensated by a model resolution, or in other words, the number of cells in the model. In horizontal projection a cell is a square or a rectangle in a simple model or irregular in a faulted model, especially in a near-fault area (Figure 2). Cell boundaries when dealing with faulted models conform to fault planes. In a vertical projection cell is a rectangle prism if the bounding is horizontal or irregular prism if they are inclined at different angles.

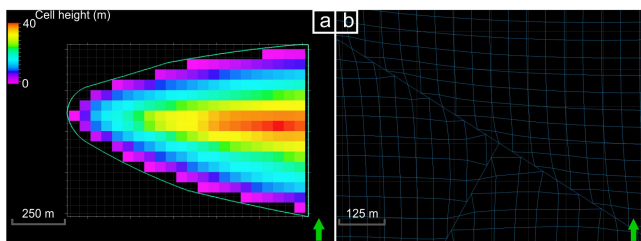


Figure 2: Horizontal cell projection in a simple (a) and faulted (b) model; color table on (a) shows cell height and the green line represents the model boundary. Cell grid is 50×50 m.

3 Comparison between numerical integration and cell-based models

At first glance many structures encountered in geology appear to be rather complex in shape. However, mostly regular geological structures can be approximated with some regular solid such as prismoid in which group accrue prism, wedge or pyramid. Volume approximated with prismoid is based on prismoidal equation

$$V = \frac{h}{6} (A_1 + 4A_m + A_2), \quad (4)$$

where h is height, A_1 and A_2 are the top and bottom areas and A_m is the area of the section situated mid-way between the end areas. The equation is correct when the figure is a

true prismoid but in practice it is applied by taking three successive cross-sections of a structure. If the mid-section is different from that of a true prismoid [10], then errors can arise. This formula is easily deduced by simply substituting areas for ordinates in Simpson's rule.

When dealing with hydrocarbon reservoir volume calculation and the structure is close to a regular anticline or syncline if stratigraphic trapping is involved, Simpson's rule is regularly applied if a number of intervals is adequate for its applicability [1]. Nevertheless, most of geological structures are irregular or faulted making a reason to simultaneously calculate volumes with Simpson's and trapezoidal rule. In this case, it is important to have in mind that calculated difference between those two methods (Eq. 5) is a criterion of method's applicability [12].

$$|I_{trap.} - I_{Simps.}| \leq 0.2I_{Simps.} \quad (5)$$

If the criterion is fulfilled then the volume calculated with Simpson's rule can be accepted as in theory, Simpson's rule is superior in defining irregular structures in the subsurface [8–10, 12].

As mentioned previously, comparison in volume calculation using trapezoidal and Simpson's rule and the ones obtained from Petrel software will be shown on four structural models; dome, elongated anticline, stratigraphic trap and faulted anticline. All ordinates for volume calculation by numerical integration ($a_0 - a_n$) were derived from Petrel model with cell size of 1×1 m ensuring that all three approaches have the same input data.

3.1 Volume calculation of a dome

Dome is a geological structure in which planes dip uniformly in all directions away from the center of the structure. In an ideal case, which is constructed here, a dome can be described as a half of a ball or a sphere. Although such a regular dome (Fig. 3) is not a realistic geological structure, it is taken into consideration as a calibration shape for selected volume calculation methods. There are ten contour lines that bound the area and which were taken in calculation and their areas are derived from Petrel software. The contour interval is 100 m. In this case Simpson's second rule or 3/8 rule is used [8, 9]. The rule is commonly used when the number of intervals is such that can be divided by three. The application of Simpson's second rule gave the volume

$$V_{Simps.} = \frac{3h}{8} \cdot (a_0 + 3a_1 + 3a_2 + 2a_3 + 3a_4 + 3a_5 + 2a_6 + 3a_7 + 3a_8 + a_9) = 2,066,776,489.86 \text{ m}^3.$$

Simpson's rule doesn't take the top of structure under calculation. Boundary of the calculation is end ordinate (a_n), thus the volume of the top above the end member is omitted from the Simpson's rule. The top of the structure can be calculated as average of two formulas [12]

$$V_{top1} = \frac{h_n a_n}{3}, \quad V_{top2} = \frac{h_n^3 \pi}{6} + \frac{a_n h_n}{2} \quad (6)$$

where h_n was the height that has to be smaller than equidistance. Here it is $h_9 = 99.99$ m, as near perfect geometry is regarded. Calculated volume of the structure top is $25,208,067.68$ m³. Consequently, the total volume of 1/2 ball calculated with Simpson's second rule was $2,091,984,557.54$ m³.

Volume calculated with trapezoidal was

$$V_{trap.} = \frac{h}{2} \cdot (a_0 + 2a_1 + 2a_2 + 2a_3 + 2a_4 + 2a_5 + 2a_6 + 2a_7 + 2a_8 + a_9) = 2,062,069,103.5 \text{ m}^3.$$

The volume derived from Petrel cell based model was $2,098,158,787$ m³. In the end, if volume of the dome – half of ball/sphere was calculated according to its usual formula

$$V = \frac{4}{3} \pi r^3 \quad (7)$$

and divided the value with 2 (hence we have the half of ball representing a dome), the yield of volume is $2,094,395,102$ m³. The value of error volume calculation by Simpson's rule is $2,410,544.460$ or 0.12% of $V_{Simps.}$, which is negligible. Given the dome is a regular structure; it is not surprising that the volume calculated by Simpson's rule gives better approximation than the trapezoidal rule. Any deviation of the Simpson's rule volume from the ideal 1/2 ball can be regarded to the possible error in the calculation of the structure top or extraction of ordinates from modelling software.

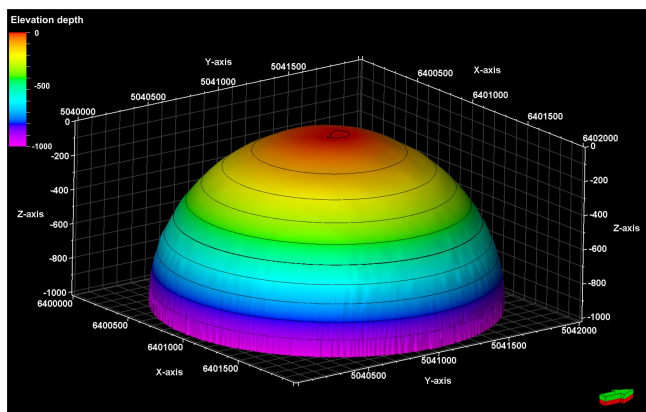


Figure 3: 3D model of dome – half of a ball/sphere derived from Petrel software.

3.2 Elongated anticline volume calculation

Elongated anticline is a fairly common structure in the subsurface, e.g. structure of the Ivanić Oil Field is a one [13]. In this case, reservoir is delimited by a structural top and oil-water contact, which is in this case at -1040 m (Figure 4). There are 7 isostrates so the Simpson's rule is applicable. Resulting volumes are fairly similar. Volume with Simpson's formula is $12,760,752$ m³, by trapezoidal rule $12,863,453$ m³ while the Petrel derived volume is $12,824,470$ m³. On this structure it is evident that trapezoidal rule gives very good volume approximation.

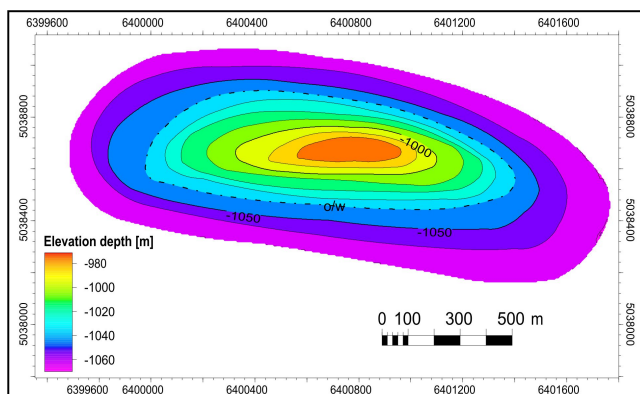


Figure 4: Structure top map (line spacing is 10 m).

3.3 Stratigraphic trap due to lateral facies change volume calculation

This kind of stratigraphic trap results when there are some variations in lithology within strata, i.e. reservoir properties are reduced in the direction of up dip and can be expected in the area without the evident structural traps but with high lateral facies change. Majority of these reservoirs are relatively thin and have an edge water contact or drive [1], thus, in practical terms, volume is calculated separately for top and bottom of the structure when using numerical integration. There are five contours which result in five ordinates or four intervals for numerical integration, thus the Simpson's rule is applicable. Structural map is shown in Figure 4 while 3D structure of trap is shown in Figure 5. Volume approximation with Simpson's rule gives value of $1,872,043$ m³, trapezoidal rule gives the volume of $1,965,020$ m³ and finally Petrel derived volume approximation is $1,917,598$ m³. The difference $V_{trap.} - V_{Simps.}$ is 5% of $V_{Simps.}$ what is acceptable by (Eq. 5).

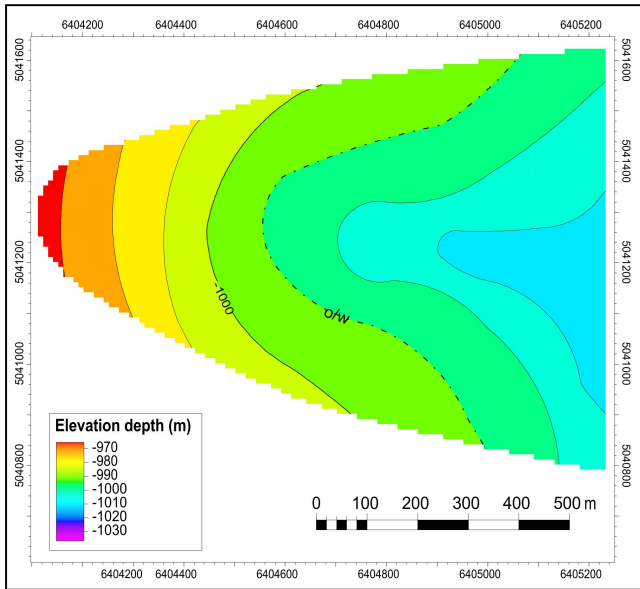


Figure 5: Top surface structure map of the stratigraphic trapping case (line spacing is 10 m).

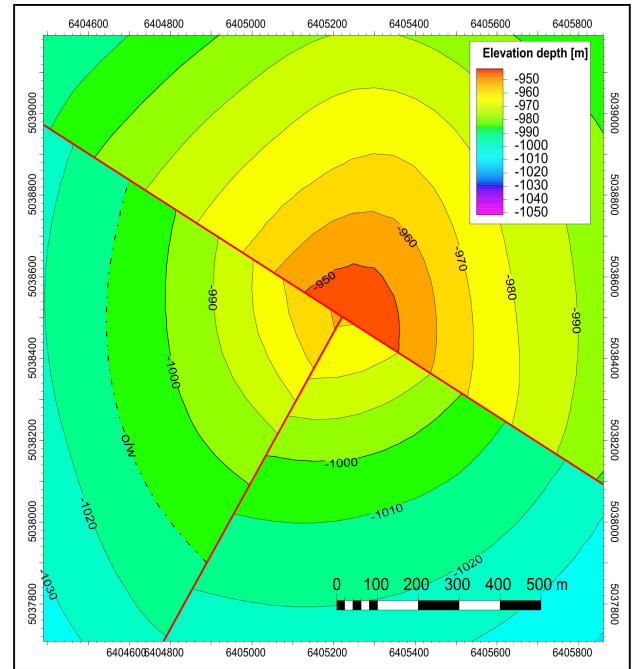


Figure 7: Reservoir top structural map (line spacing is 10 m).

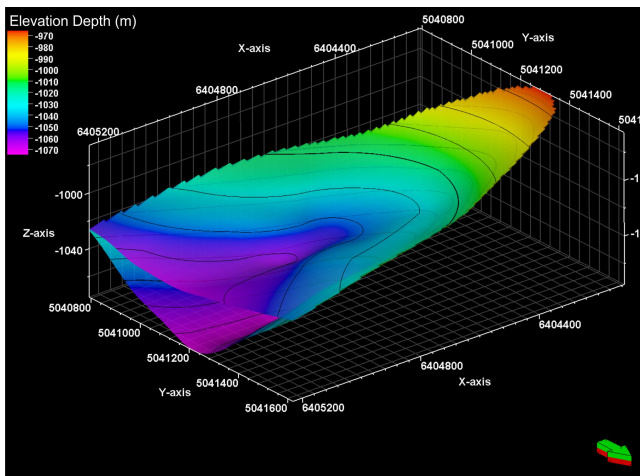


Figure 6: 3D model of stratigraphic trap derived from Petrel software.

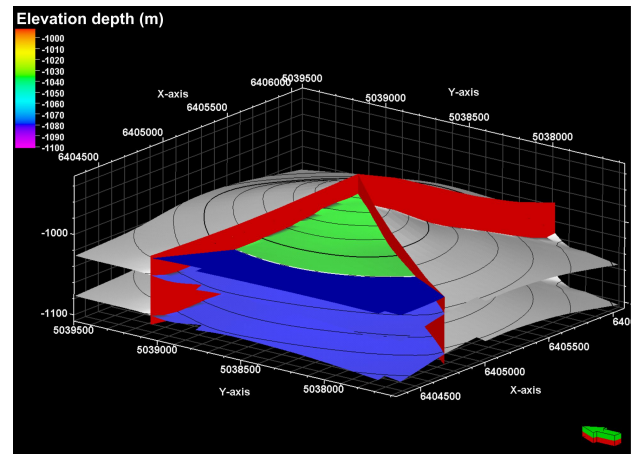


Figure 8: 3D model of faulted anticline trap derived from Petrel software; volume calculation refers only to the green colored part of the model.

3.4 Faulted Anticline volume calculation

The last example of reservoir volume calculation was the faulted anticline shown at Figure 6 & 7. The reservoir was delimited by structural top, two normal faults and fluid's contact. There are five contour lines that describe the reservoir. Application of Simpson's rule gave the value of 4,276,883 m³ and by trapezoidal rule a volume of 4,409,083 m³. Petrel derived volume gives was 4,372,932 m³. Simpson's rule volume gives underestimated value and trapezoidal rule overestimated in comparison to model derived one.

4 Cell based volume calculation and grid resolution

In theory, cell based model calculation can be made with very high resolutions but in practical terms, an optimal grid size has to be taken. Bulk volume by itself is a no problem for today's computers, but later procedures (e.g. petrophysical modelling) which take into the account the resolution of the initial model will be too detailed for calculation.

Table 1: Presentation of calculated bulk volumes for each cell size with the relation of cell area to the calculated volume area and the difference in calculated volumes to the maximum resolution case.

Grid cell size (m)	bulk volume (m ³)	cell surface to structure surface ratio (%)	calculated volume to 1 × 1 grid volume ratio (%)
1 × 1	1,917,598	0.0003	0
2 × 2	1,917,419	0.001	0.0093
5 × 5	1,916,164	0.008	0.0748
10 × 10	1,905,282	0.032	0.6423
20 × 20	1,885,545	0.129	1.6715
50 × 50	1,759,308	0.812	8.2546
100 × 100	1,403,102	3.249	26.8303
200 × 200	777,488	12.997	59.4551

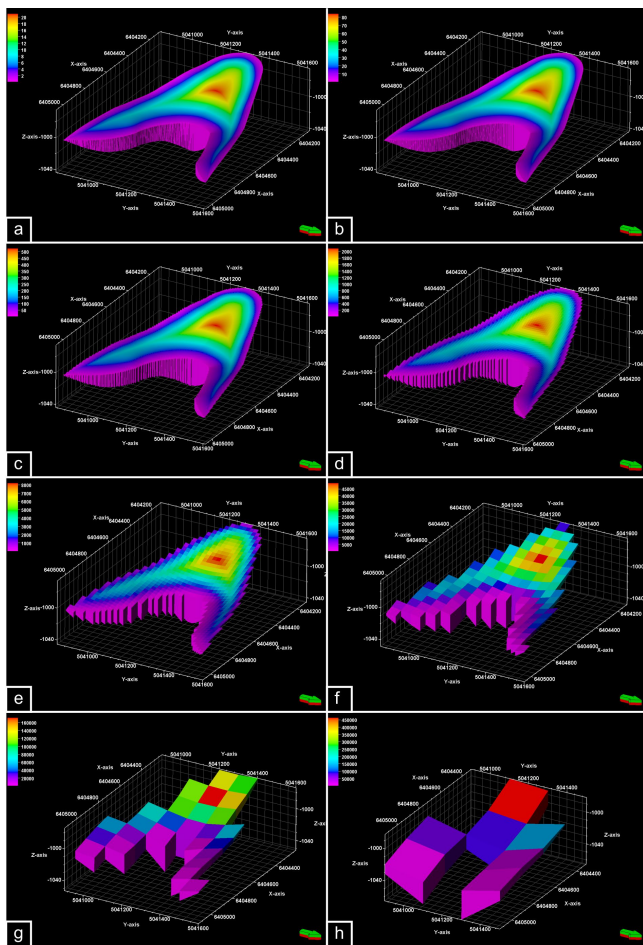


Figure 9: Representation of the impact of cell grid size on the model detail and smoothness for 1 × 1 (a), 2 × 2 (b), 5 × 5 (c), 10 × 10 (d), 20 × 20 (e), 50 × 50 (f), 100 × 100 (g) and 200 × 200 (h); color legend represents cell volume in m³.

For this purpose, eight models of previously described stratigraphic trapping case (Figure 4 & 5) were taken into the account of lateral grid resolution (cell size) 1, 2, 5, 10,

20, 50, 100 and 200 m for structure area of 307,749 m². The difference in cell size and grid smoothness can be clearly observed in Figure 9. Detail coverage of the reservoir area was obtained with highest resolution (1 × 1 m cell) in Figure 9a while very rough cell coverage can be observed when grid size exceeds 50 m (Figure 9g & 9h). The calculated model volume for each cell size is presented in Table 1.

5 Discussion

Volumes calculated by all three approaches differ slightly (Table 2). These differences are of about 0,2% for dome – 1/2 ball/sphere, 0,4–0,8% for anticline and around 2–5% for stratigraphic trap and faulted anticline cases. It can be observed that these values are not even near the 20% difference for confirming the validity of volume calculation between the Simpson's and Trapezoidal approach stated in (Eq. 5) stated in [12].

Grid resolution is a key factor when cell based models are observed, Volumes differ very little in high resolution cases – only up to 1.6% for cells smaller than 20 × 20 m, *i.e.* when single cell area is not larger than 1.7% of the whole structure area. Large differences (> 5%) occur for 20 × 20 or larger cells, when single cell covered 1.7–8.3% of the structure area. These differences can also be called errors derived from low resolution. There is no rule of thumb in how much of a volume difference or error is acceptable but it would be advisable to keep it below 1% for high resolution models or 5% when a high resolution is not needed (usually used in early stage of the modelling). The 1% margin would correspond to the grid size of 0.0008% of the structure area or approximately 15 × 15 m cell grid and 5% to 0.0035% or a 30 × 30 m cell grid for the described case (Figure 10).

Table 2: Bulk volume calculation results for all cases.

Case	$V_{\text{Simpson's rule}} \text{ (m}^3\text{)}$	$V_{\text{trapezoidal rule}} \text{ (m}^3\text{)}$	$V_{\text{structure top}} \text{ (m}^3\text{)}$	$V_{\text{Simpson's rule with added structure top}} \text{ (m}^3\text{)}$	$V_{\text{trapezoidal rule with added structure top}} \text{ (m}^3\text{)}$	$V_{\text{cellmodel}} \text{ (m}^3\text{)}$	
Dome - 1/2	2,066,776,489	2,062,069,103	25,208,067	2,091,984,557	2,087,277,171	2,098,158,787	
Ball/sphere							
Elongated anticline	12,648,184	12,750,885	112,568	12,760,752	12,863,453	12,824,470	
Stratigraphic trap	Reservoir base	1,972,293	2,051,065	8,347	1,872,043	1,965,020	1,917,598
	Reservoir top	3,829,008	4,000,757	23,675			
Faulted Anticline	4,250,501	4,382,702	26,381	4,276,883	4,409,083	4,372,932	

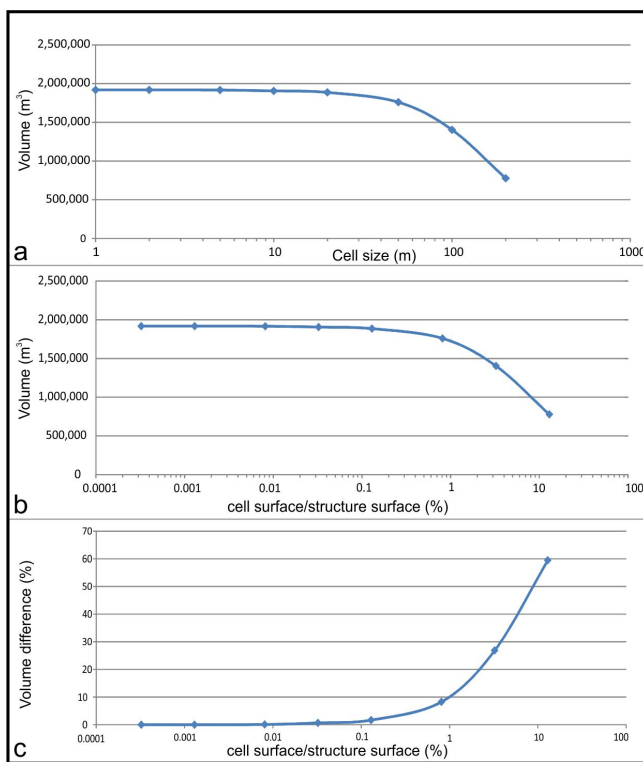


Figure 10: Graphs showing the relation of the grid cell size and calculated volume (a), cell area to structure volume area relation against calculated volume (b) and cell area to structure volume area relation against volume difference between volumes of the calculated case to the maximum resolution one (c).

As an example, for modeling petrophysical parameters for the assessment of reservoir performance a cell grid area of 0.0011% (50 × 50 m over an area of 1500 × 1000 m) can be used but this is not thoroughly enough for the later representation of the detailed sedimentary structures [14].

For instance, for development of old, nearly depleted oil fields a high resolution model is often used. As an example, for sequence stratigraphic analysis and integrated 3D modelling of such, a very dense grid of 20 × 20 m covering the area of 6.84 km² is used [15]. These values correspond to a cell to model area size relation of 0.0058% or the possible volume difference of only 0.05%. These are very detail explorations when high resolution facies distribution is needed when searching for compartmented and bypassed oil. As another example, calculation of volumes when regarding cell size is not restricted to hydrocarbons, but is also to be regarded when dealing with CO₂, as well as for storage purposes and possibility of seepages through detail modelling [16].

Volume calculation of prospects in a regional study is highly susceptible to large difference in the actual volume in place. For instance, due to the large area of modelling, cell size is relatively large (e.g. 100 × 100 m for an area of 340 km² as in [17]). For small size prospects (e.g. horizontal projection area of 0.5 km²) cell to model area size relation is large (2%) which as a result can have an underestimation of the initial bulk volume by almost 20%.

6 Conclusions

In all presented examples of reservoir volume calculation (Table 2) it was obvious that Simpson's rule shows better results when structure is close to a regular anticline (dome) but in all other structures it gives the underestimated value compared to the cell based model volume. The trapezoidal rule gives good results when structure was

irregular and shows the values which are close to high resolution cell based model, although they were in all cases overestimated with exemption when dome was regarded. It is also important to emphasize that Simpson's rule can't be taken under consideration when the number of ordinates or isopach contours is even (apart from the Simpson's second rule) thus making the Trapezoidal most practical for use. Approximations of Simpson's rule which allow the use of even number of ordinates however do exist [18] but were not taken into the consideration in this investigation. Even with relatively small number of ordinates or isopach contours, both numerical integration methods gave very good results when compared to the detailed cell based model, thus once again confirming their applicability in the volume calculation process.

When using modeling software for volume calculation, model resolution plays the key part. As the grid resolution decreases the volume calculation suffers from a decline in calculated volumes (Table 1). The largest errors occur after crossing the threshold when the area of the cell surpasses the 0.0035% of the reservoir area or a 5% difference in volume. For later purposes it is advisable that the cell area of the model is not larger than 0.0008% of the reservoir area. Cell to model area size relation is very important in regional studies (e.g. basin modelling) when the cell size is adjusted for the entire model area. In these cases underestimation of possible hydrocarbon volumes can occur in the scale of 20% or more depending on the prospect and cell size.

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