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## Methodological aspects of hydrocarbon shale resources assessment using different variants of volumetric methods

The article presents the methodological aspects of hydrocarbon resources calculation accumulated in shale formations using two variants of the volumetric method based on different data sets. The first method constitutes an extension of the classic volumetric method taking into account adsorbed gas presence on kerogen surface. This method can be applied to formations saturated with oil, condensate, as well as dry gas. The second proposed method can be used for resources calculations in oil-saturated reservoirs only. It involves the use of geochemical data (Rock Eval pyrolysis data), results of PVT measurements of reservoir fluids and Langmuir isotherm. The possibility of using different methodological approaches allows to carry out calculations in different conditions of data availability. Both methods, used for test calculations of hydrocarbon resources in oil type shales, give surprisingly consistent results.

Key words: resources, volumetric calculation method, shale formation, geological model.

### Aspekty metodyczne szacowania zasobów węglowodorów z formacji łupkowych obliczanych metodą objętościową

W artykule przedstawiono metodologiczne aspekty obliczenia zasobów węglowodorów zakumulowanych w skałach łupkowych wykorzystując dwa warianty metody objętościowej bazujące na odmiennych zestawach danych. Pierwszy wariant stanowi rozszerzenie klasycznej metody objętościowej i uwzględnia charakterystyczną dla złóż typu *shale*, obecność gazu zaadsorbowanego na powierzchni kerogenu. Ta metoda obliczeń może być stosowana dla stref nasyconych ropą naftową z gazem rozpuszczonym w ropie, stref występowania kondensatu, jak również dla formacji nasyconych suchym gazem. Drugi wariant umożliwia prowadzenie obliczeń zasobów węglowodorów niekonwencjonalnych jedynie w złożach ropnych i bazuje na danych geochemicznych (Rock Eval), wynikach analiz PVT mediów złożowych oraz wyznaczonej laboratoryjnie izotermie Langmuir'a aplikowanej w celu oszacowania ilości gazu adsorbowanego. Możliwość stosowania odmiennych podejść metodycznych pozwala na prowadzenie obliczeń w różnych uwarunkowaniach dostępności danych. Wykorzystanie obu wariantów metodycznych dla testowych obliczeń zasobów geologicznych w złożu ropnym, dało w rezultacie stosunkowo zbieżne wyniki.

Słowa kluczowe: szacowanie zasobów, metoda objętościowa, formacje łupkowe, model geologiczny.

### Introduction

Literature references regarding to the methodology for estimation of unconventional resources accumulated in shale formations (gas shales/oil shales) indicate several methodological approaches. These approaches have been developed for the purpose of analyzing resources at various stages of exploration, development and exploitation of unconventional oil and gas reservoirs. Therefore, there are significant differences

due to the types of geological, geochemical, petrophysical and reservoir data used. Generally, methods for estimating hydrocarbon resources in shale formations can be divided as follows [1, 5, 7, 9]:

- volumetric methods (calculation based on maps and reservoir models),
- material balance method (approach based on effects of

analysis of generation and distribution of hydrocarbons in source rocks),

- production history (based on production data analysis),
- analogy (based on comparative analysis with similar reservoir which is well explored).

At the current stage of exploration of unconventional reservoirs in Polish shale formation, the most appropriate for

resources calculation, is the volumetric calculation method. In this article two approaches for conducting calculations of resources using high resolution geological model have been subjected and developed.

The proposed methodology has been tested on dataset from a shale oil reservoir containing dissolved gas (unsaturated oil reservoir).

### Pore space characterization

Before any discussion relating to the calculation of resources, it is important to understand the elements composing hydrocarbon bearing shale rocks. An essential element distinguishing shale oil/gas reservoirs from a conventional reservoir constitutes accumulation of hydrocarbons in source rock where it was generated. Therefore, source rock acts as reservoir rock and seal where mobility of hydrocarbons takes place on a small scale (micro) or is absent. Below in the scheme proposed by Eslinger and Everett [4] (Figure 1) model of the presence of particular components in this type of rock is shown.

Hydrocarbon-bearing shale formation consists of matrix (organic and non-organic), water (free, bound, irreducible) and hydrocarbons (oil and gas). The presence of fluid components including water and hydrocarbons is divided into the following porosity types: bound water porosity, irreducible fluids porosity,

free porosity [4]. The sum of these three constitutes total porosity. The difference between total and effective porosity is bound water porosity which always occurs in shale rocks. The petrophysical characteristics of shale formation is defined generally as extremely small pores and low permeability which implicates the need for accurate measurement of these two parameters. The nano scale pores, which were formed as a result of organic matter maturation, can form a major pore space for shale hydrocarbon storage. The presence of adsorbed gas, which characterizes hydrocarbon-bearing shale formations, causes the need to extend standard volumetric method (used for conventional reservoirs) which would allow, to take adsorbed gas into account as well. Most of this gas is generally assumed to be adsorbed to kerogen, whereas the volume of adsorbed gas, depends on the type of kerogen, gas component and sorption capacity [4].

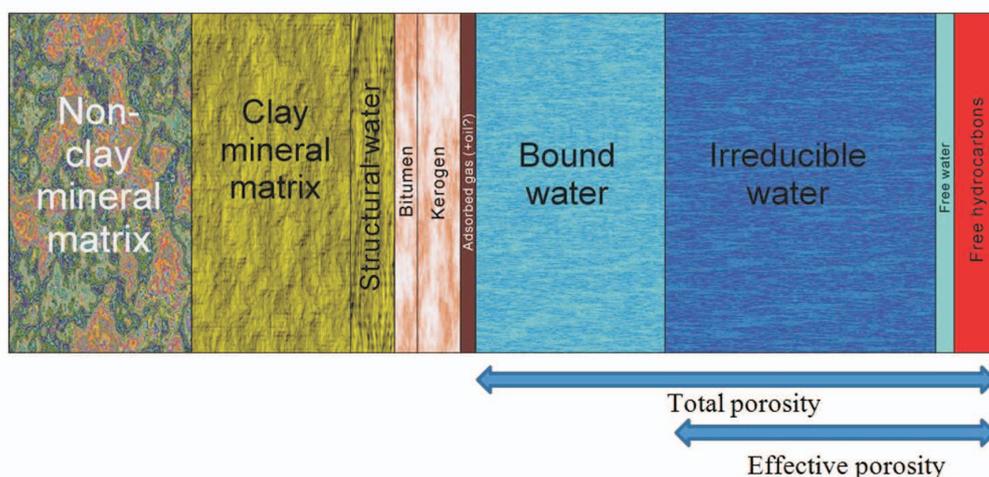


Fig. 1. Model used for interpretation of shale formation components along wellbores [4]

### The extension of the standard volumetric method of hydrocarbon in place calculation to account for adsorbed gas

This procedure to a certain degree is analogous to the approach used in conventional resources calculation; oil resources in oil reservoir (STOIP) and gas resources in gas reservoir (GIIP) are calculated according to the formula describing the volume of effective pore space in a certain

volume of reservoir, reduced by the volume of water. Formation volume factor of oil ( $B_o$ ) and gas ( $B_g$ ) determined by PVT measurements of reservoir fluids, converts the volume of hydrocarbons from reservoir to surface conditions. The following formulas can be used accordingly for oil saturated

zones with dissolved gas, condensate occurrence zones as well as for the formations saturated with dry gas [1, 5]:

$$STOIP_{I1} = \frac{V \cdot \phi_{eff} \cdot (1 - Sw)}{B_o}$$

$$GIIP_{in\_oil\_I1} = STOIP \cdot R_s = \frac{V \cdot \phi_{eff} \cdot (1 - Sw)}{B_o} R_s$$

$$GIIP_{I1} = \frac{V \cdot \phi_{eff} \cdot (1 - Sw)}{B_g}$$

STOIP<sub>I1</sub> – Stock Tank Oil Initially In Place [m<sup>3</sup>] in oil reservoir,  
 V – volume of reservoir [m<sup>3</sup>],  
 φ<sub>eff</sub> – effective porosity,  
 Sw – water saturation,  
 B<sub>o</sub> – formation volume factor of oil,  
 GIIP<sub>in\_oil\_I1</sub> – volume of dissolved gas in oil [m<sup>3</sup>],  
 R<sub>s</sub> – gas–oil ratio,  
 GIIP<sub>I1</sub> – Gas Initially In Place [m<sup>3</sup>] in gas reservoir,  
 B<sub>g</sub> – formation volume factor of gas.

The aforementioned formulas are widely known ways for the calculation of oil and gas resources which fill pore space of conventional reservoirs. When applied to unconventional reservoirs they allow to calculate volumes of oil and/or gas present in the form of free oil/gas. As it was mentioned before the adsorption phenomena of kerogen occurs in unconventional reservoirs of oil/gas shales next to hydrocarbons in free form. The amount of adsorbed gas depends on, among others, the amount of organic matter occurring in rock and thermal maturity; according to Jarvie [6] in U.S. shale reservoirs, the amount of adsorbed gas can range from 10÷70% of total gas.

Mentioned extension of the standard volumetric method involves taking adsorbed gas into consideration. The volume of adsorbed gas is determined using the Langmuir isotherm defining the sorption capacity of the rock under a specified pressure and at a constant temperature (Figure 2).

Langmuir isotherm allows to determine the sorption capacity at given pressure conditions of the reservoir

being analyzed. Sorption capacity is calculated through the following formula [8]:

$$V_s = \frac{VL \cdot p}{pL + p}$$

V<sub>s</sub> – sorption capacity [m<sup>3</sup>/t],  
 VL – Langmuir sorption capacity [m<sup>3</sup>/t],  
 pL – Langmuir pressure – pressure at  $\frac{VL}{2}$  [MPa],  
 p – reservoir pressure [MPa].

Assuming that the total sorption capacity is filled with gas, the volume of gas adsorbed in the reservoir is calculated as following:

$$GIIP_{adsorbed} = V \rho_{rock} V_s$$

GIIP<sub>adsorbed</sub> – volume of adsorbed gas in shale type reservoirs of hydrocarbons [m<sup>3</sup>],  
 ρ<sub>rock</sub> – rock density [t/m<sup>3</sup>].

In this approach the total amount of hydrocarbons in place is the sum of those occurring in the form of free oil/gas, gas dissolved in oil and gas adsorbed on the surface of kerogen.

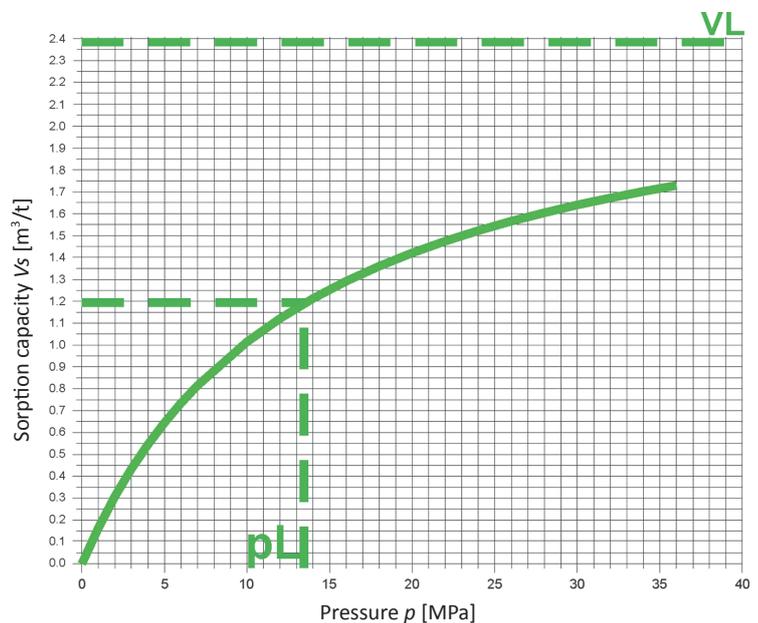


Fig. 2. Example of Langmuir isotherm

**Method of shale resources assessment based on geochemical data, PVT data and Langmuir isotherm**

The second method for calculating resources of shale formation is based on geochemical data, results of PVT measurements of reservoir fluid samples and Langmuir isotherm.

This method can be implemented only for oil saturated reservoirs (oil shales) and does not require models of spatial

distribution of porosity and water saturation. Estimation of the oil volume is carried out based on the S1 parameter values indicating the amount of liquid hydrocarbons accumulated in rock. Since the measurements are made on samples of milled rock, they are free of the lightest hydrocarbons (C<sub>1</sub>–C<sub>5</sub>) which

constitute the gas phase (dissolved gas in the crude oil or as a free gas phase) and the S1 parameter indicates the amount of oil [mg HC/g rock] or [kg HC/tonne rock] therefore this method cannot be applied for reservoirs saturated by dry gas.

The volume of oil in shale formation can be estimated based on three variants of this method:

- using quantitative laboratory indicators of bituminous extract from shale formation core samples,
- using results of Rock Eval pyrolysis analysis (S1),
- using results of Rock Eval pyrolysis analysis compared with hydrocarbon solvent extraction [3].

The first variant involves the extraction of hydrocarbons contained in the sample by leaching them using particular organic solvents; after evaporation of the solvent at 60°C temperature, determination of the extract amount is carried out. The asset of this method is little effort while the disadvantage, a relatively high estimation error reflected in the declination of lighter fractions (volatile) of extracted hydrocarbons during the solvent evaporation process. It causes the underestimation of the hydrocarbons amount.

Assessment of liquid hydrocarbons using the second variant is based on S1 [mg HC/g rock] parameter which is determined in Rock Eval pyrolysis process. Determination of S1 is the simplest way to assess the amount of hydrocarbons in rock but it is also encumbered with an error. The S1 parameter it is an amount of free liquid hydrocarbons contained in the pore spaces of rocks which are released from the sample. Error stems from the fact that the S1 parameter expresses the amount of free liquid hydrocarbons contained in the rock, released during pyrolysis at temperatures up to 300°C which constitutes only part of the total amount of liquid hydrocarbons. A certain portion of the heavier fractions of crude oil, can be released at higher temperatures (Figure 3).

Much more reliable but also more time consuming is the third variant based on the pyrolysis Rock-Eval analysis referred to as hydrocarbon extraction. It consists of double determination of hydrocarbons of the same sample, whereupon the first analysis is held before hydrocarbon extractions, and the second after extraction. Calculations are based on S1 and S2 parameters. The S2 parameter indicates the amount of hydrocarbon released under temperatures ranging from 300 to 650°C. It is a reflection of residual hydrocarbon potential of source rock, which can generate hydrocarbons. The potential of high thermal matured hydrocarbon-bearing rock can be associated with heavy fractions of generated hydrocarbons

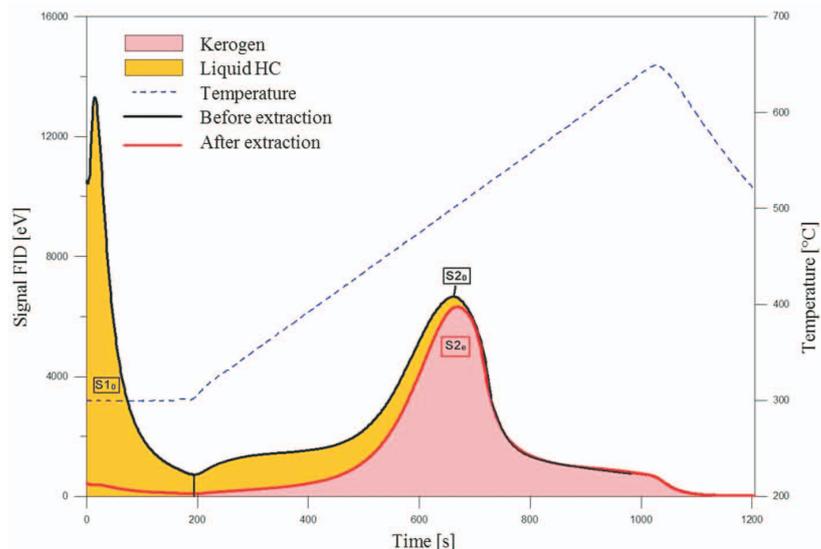


Fig. 3. Results of Rock Eval pyrolysis experiments showing the characteristics of S1 and S2 picks of a shale rock sample before (black line) and after (red line) extraction (experiments were carried out in INiG – PIB)

before expulsion. This part of oil is represented by unsaturated fractions of hydrocarbons in the range of  $nC_{18}$ – $nC_{35}$ , which boiling point exceeds 300°C while hydrocarbons releasing is continuous up to 450°C (Figure 3). The amount of liquid hydrocarbons calculated using this variant is determined according to the following formula:

$$HC = S1_0 + (S2_0 - S2_e)$$

where:

HC – amount of liquid hydrocarbons contained in rock [mg HC/g rock],

$S1_0$  – value of S1 parameter before bituminous extraction [mg HC/g rock],

$S2_0$  – value of S2 parameter before bituminous extraction [mg HC/g rock],

$S2_e$  – value of S2 parameter after bituminous extraction [mg HC/g rock].

Each of the presented methods have particular disadvantages. In the first method, the amount of hydrocarbons is underestimated due to light fractions loss ( $C_1$ – $C_5$ ) during solvent evaporating. In the second method, the reason for the underestimation is the omission of a significant part of heavy fractions (released over 300°C). The third variant is the most reliable but on the other hand, time consuming. This variant requires double pyrolysis analyzes of the same sample before and after bitumen extraction.

Considering the limitations of each variant for the determination of total liquid hydrocarbons amount, attempts to define S1 have been made. It comes down to the evaluation of correlation between value of any parameter from Rock

Table 1. Amount of hydrocarbons measured by 3 variants

Variant	I [ppm]	II [ppm]	III [ppm]	<i>r</i> (III/II)
Sample 1	2082	1570	2720	1.73
Sample 2	3275	2400	3600	1.50
Sample 3	3017	1670	2900	1.74
Sample 4	4583	2660	5090	1.91
Sample 5	3893	2470	3990	1.62
Sample 6	4172	2420	4780	1.98
Sample 7	1654	1280	2230	1.74
<i>r</i> average:				1.75

Eval pyrolysis and the value of ΔS2. Laboratory experiments performed on 7 samples representing the most potential Polish shale formations indicate good correlation between results based on calculation by the second and third variants. For all samples which thermal maturity *T<sub>max</sub>* is in the range of 457÷463°C, the amount of liquid hydrocarbons calculated by the third variant is proportional to the results of the second method. Correlation coefficient between these two results is 0.86 and proportional ratio (*r*) is in the range of 1.50÷1.98 while its average is equal to 1.75.

$$S1_0 \cdot r = S1_0 + (S2_0 - S2_e)$$

*r* – proportional ratio – amount of hydrocarbons measured in III variant divided by amount of hydrocarbons measured in II variant. It is used to scale *S1<sub>0</sub>* data into *S1 + (S2<sub>0</sub> – S2<sub>e</sub>)* form without the need to carry out additional extraction and pyrolysis experiments.

Thus, for volume determination of oil in shale formation calculated based on pyrolysis results, proportional ratio “*r*” needs to be considered. It should also be noted that the value of *r* parameter is strongly dependent on the thermal maturity of rock.

Since the measurements are made on samples of ground rock, they are devoid of the lightest hydrocarbons (C<sub>1</sub>–C<sub>5</sub>), which constitutes gas in the reservoir (dissolved in oil or

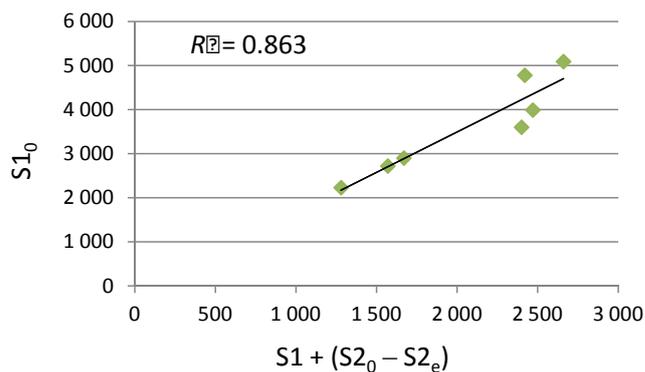


Fig. 4. Correlation graph of the amount of total liquid hydrocarbons versus *S1<sub>0</sub>* parameter

free gas). Accordingly, this method cannot be used for dry gas reservoirs. Determination of the volume of oil in shale formations for particular interval and defined geometry is calculated as follows:

$$STOIP_{II} = \frac{V \cdot \rho_{rock} \cdot S1 \cdot r}{\rho_{oil}}$$

STOIP<sub>II</sub> – Stock Tank Oil Initially In Place [m<sup>3</sup>] calculated by second method,

*S1* – amount of hydrocarbons [kg HC/t],

*ρ<sub>oil</sub>* – oil density [kg/m<sup>3</sup>].

Volume of dissolved gas in oil (GIIP<sub>in\_oil\_II</sub>) can be calculated analogously as in the first approach presented above:

$$GIIP_{in_oil_II} = STOIP_{II} \cdot R_s$$

GIIP<sub>II</sub> – Gas Initially In Place [m<sup>3</sup>] calculated by second method.

Similarly, calculation of hydrocarbons volume held by adsorption forces is carried out with the same formula:

$$GIIP_{adsorbed} = V \cdot \rho_{rock} \cdot V_S$$

The total amount of hydrocarbons in place is the sum of those occurring in the form of free oil/gas, gas dissolved in oil and gas adsorbed on the surface of kerogen.

### Estimating resources using a high resolution geological model

For possible accurate assessment of hydrocarbon resources accumulated in shale formation it is necessary to build a static property model of 3D distribution of crucial parameters involved in the calculations such as effective porosity, Total Organic Carbon (TOC), water saturation, and rock density. 3D models of reservoir properties used for calculation of shale resources allow to present its results as a 3D distributions

of STOIP, GIIP, GIIP<sub>in\_oil</sub>, and GIIP<sub>adsorbed</sub> within reservoir to be used for: interpretation of intervals with the greatest hydrocarbon potential, designation of the most prospective areas within the field, supporting wells trajectory design or economic analyzes [12]. The scheme on next page (Figure 5) shows a geomodeling workflow which was applied to the dataset prior to volumetric calculations.

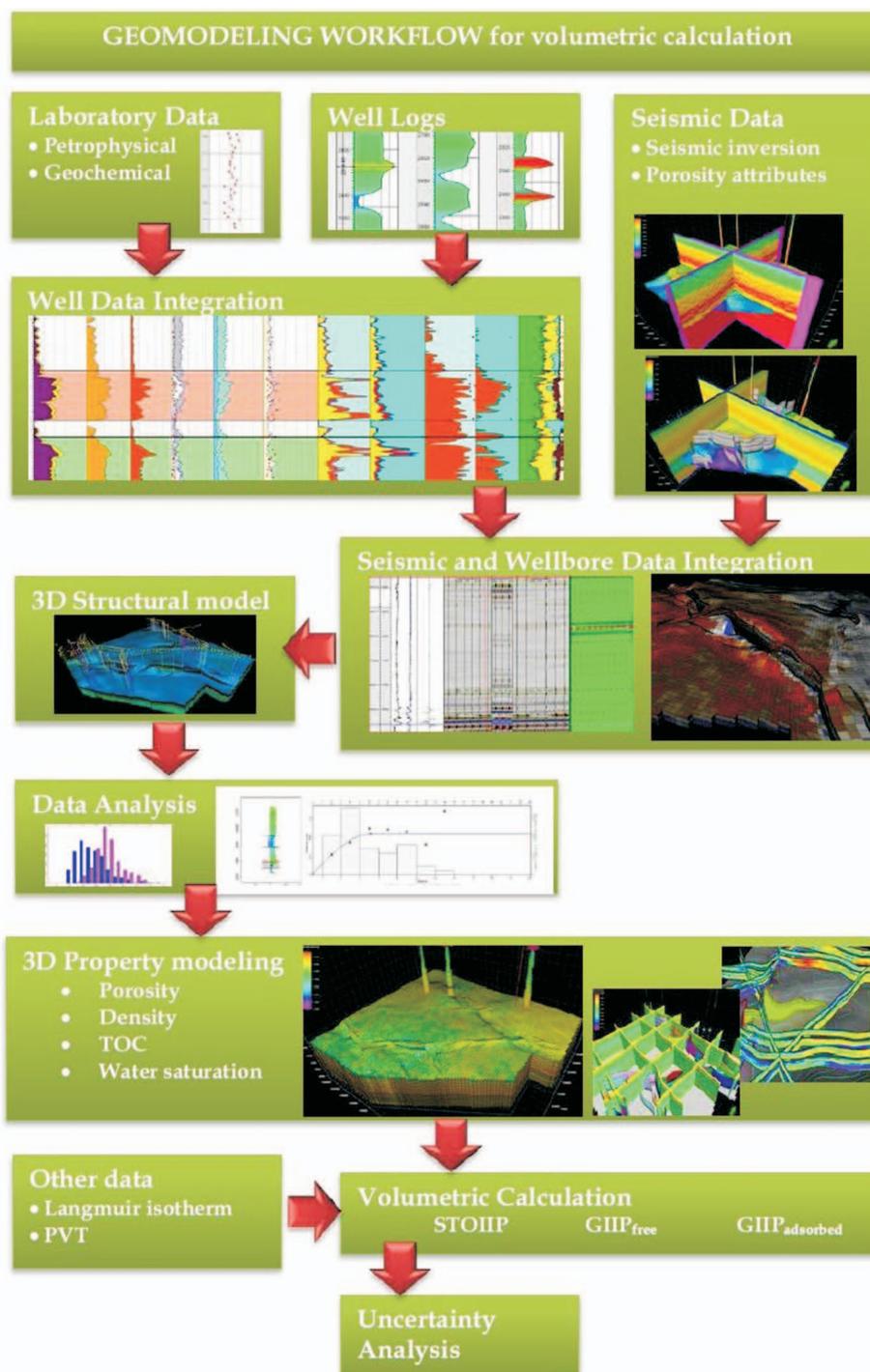


Fig. 5. Scheme of geomodelling workflow which was carried out for resources estimation based on 3D models of shale formation

### Calculation

For the purpose of testing the proposed methodology for the calculation of hydrocarbon resources in shale formations, a geological model including selected shale interval with resource potential was created. The volume of each reservoir fluid was calculated on the basis of parametric models including the spatial distribution of the following parameters:

- effective porosity and water saturation (for calculation of resource by I method),
- rock density (for the calculation of the adsorbed gas volume within model volume; for method I and II),
- TOC as the property supporting determination of the spatial distribution of S1 parameter (for the II method). Methodologies developed for resource calculation are

applied in every cell (i) of the created model. The only constant values for the calculation by first approach are the thermodynamic parameters  $B_o$  and  $R_s$ . In the second method, constant parameters are proportional ratio  $r$ , oil density and oil-gas ratio  $R_s$ .

The use of methods described above (utilizing different set of data) for test calculations gave surprisingly similar results. Hydrocarbon resources of shale rocks calculated by method I constitute 95.5% of the resources calculated by method II.

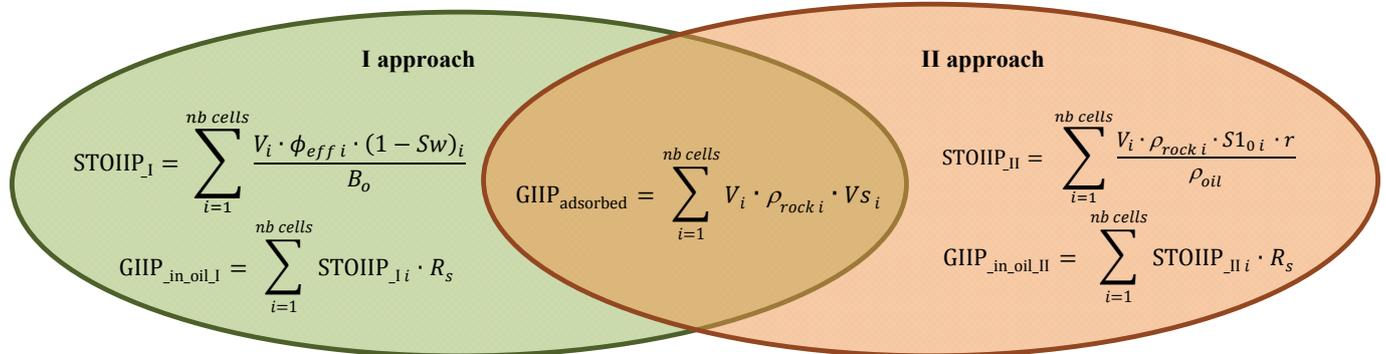


Fig. 6. Proposed methods for shale oil/gas resources assessment

where:

- STOIIP – Stock Tank Oil Initially In Place [m<sup>3</sup>] in oil reservoir,
- $V$  – volume of reservoir [m<sup>3</sup>],
- $\phi_{eff}$  – effective porosity,
- $Sw$  – water saturation,
- $B_o$  – formation volume factor of oil,
- $GIIP_{in\_oil}$  – volume of dissolved gas in oil [m<sup>3</sup>],
- $R_s$  – gas–oil ratio,
- $GIIP_{I,II}$  – Gas Initially In Place [m<sup>3</sup>] in gas reservoir,
- $GIIP_{adsorbed}$  – volume of adsorbed gas in shale reservoirs [m<sup>3</sup>],

- $\rho_{rock}$  – rock density [t/m<sup>3</sup>],
- $VS$  – sorption capacity [m<sup>3</sup>/t],
- $S1_0$  – value of S1 parameter before bituminous extraction [kg HC/t rock],
- $r$  – proportional ratio – amount of hydrocarbons measured in III variant divided by amount of hydrocarbons measured in II variant. It is used to scale  $S1_0$  data into S1 + (S2<sub>0</sub> – S2<sub>c</sub>) form without the need to carry out additional extraction and pyrolysis experiments,
- $\rho_{oil}$  – oil density [kg/m<sup>3</sup>].

### Summary

The main purpose of this article was to evaluate the theoretical and methodological aspects of shale formation hydrocarbon resources assessments, conducted with a 3D model of the reservoir using the volumetric method. Two methods of calculating resources of hydrocarbons accumulated in shale formation obtaining consistent results have been developed. The advantage of the possibility of using different methodological approaches, is that they require a slightly different set of data which entail the possibility of calculation of disparate stages of data availability. The main conclusions obtained:

1. The main difference between conventional reservoirs and shale formation is the occurrence of adsorbed gas which can be determined by the Langmuir isotherm.
2. For estimating the volume of particular hydrocarbons two different methods were developed. The first method cover reduction of pore space by water and the addition

of adsorbed gas, the second approach involves calculation of the volume of oil and dissolved gas based on the S1 parameter from Rock Eval pyrolysis and the addition of the adsorbed gas.

3. The first method can be used for resources assessment of oil, gas and condensate reservoirs, the second method can be used only to assess oil resources in oil shales. Both methods require different types of data.
4. For accurate volumetric calculation of hydrocarbon resources a high resolution 3D model is required to create spatial distribution of parameters significant for this calculation.
5. Calculations of hydrocarbons volumes made by proposed methods gives surprisingly similar results.
6. The methodology can be easily implemented but the credibility of results, hinges on appropriate assumptions and proper data to represent heterogeneity of the reservoir.

Please cite as: Nafta-Gaz 2015, no. 6, pp. 400–407

Article contributed to the Editor 26.02.2015. Approved for publication 15.04.2015.

The article was based on research study entitled: *Dostosowanie objętościowej metody obliczania zasobów złóż gazu z formacji łupkowych* – INiG – PIB, ordered by MNiSW. Archival number DK-4100-43/14.

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