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Implementation of petroleum system modeling technique in shale gas resources assesment

The article presents petroleum system modeling technique application for prognostic hydrocarbons resource assessment which takes into account hydrocarbon retention process within source rocks. For that purpose, during the modeling, source rocks kerogen sorption parameters have been defined, based on laboratory measurements of analyzed shale layer. One dimensional modeling have been conducted for one well profile located in the Baltic basin. Results shows a great impact of taking into consideration adsorption process, on proper hydrocarbon balance calculation in an analyzed petroleum system.

Key words: modeling, shale gas, adsorption.

Implementacja metod modelowania systemów naftowych do obliczania zasobów złóż w formacjach łupkowych

W pracy przedstawiono metodykę modelowania systemów naftowych dla obliczania prognostycznych zasobów węglowodorów metodą genetyczną z uwzględnieniem procesu akumulacji węglowodorów w skale macierzystej. W tym celu w trakcie modelowania określono parametry sorpcyjne kerogenu występującego w skale macierzystej i dokonano obliczenia bilansu węglowodorowego dla warstwy skał łupkowych. W celu określenia modelu sorpcji węglowodorów w skale macierzystej wykorzystano dostępne wyniki badań laboratoryjnych. Jednowymiarowe modelowanie zostało przeprowadzone w profilu otworu zlokalizowanego w basenie bałtyckim. Wyniki modelowania wskazują na konieczność uwzględnienia procesów akumulacji węglowodorów w skale macierzystej w celu poprawnego obliczenia bilansu węglowodorowego w analizowanym systemie naftowym.

Słowa kluczowe: modelowanie, gaz łupkowy, adsorpcja.

Introduction

In a new era of unconventional shale gas exploration, there is a need for modification and improvement of the techniques used so far in conventional oil and gas exploration.

The aim of this work is to present the methodology for calculating the prognostic hydrocarbon resources, by a genetic method that takes into account numbers of hydrocarbons accumulated within source rocks of existing petroleum play. Methodology improves hydrocarbon balance calculation by taking into account source rock HC retention processes – in this case, Ordovician shale layer has been analyzed as a simultaneous source and reservoir rock. This improvement has been reached by source rock sorption capacity model implementation.

The whole assessment is proceeded by numerical technique called petroleum system modeling.

The aim of this work was the analysis of petroleum system modeling technique application in petroleum systems with shale plays. One dimensional modeling was conducted for one well, located in the Baltic basin (northern Poland) which is a major target for shale gas exploration [7].

Petroleum system modeling – technique and workflow

Petroleum system modeling (basin modeling) is a technique which refers to numerical modeling of physical and chemical processes which take place in sedimentary basins leading to oil and gas accumulations formation [5]. This method was developed in the 80s. At the end of the 90s, the first spatial simulation of petroleum processes was carried out [4]. One of the pioneering work in this field is that of D. H. Welte and M. A. Yükler *Petroleum origin and accumulation in basin evolution – A quantitative model* published in 1984 [16]. Today, this technique is routinely used in exploration and in scientific works.

Petroleum system modeling is a dynamic modeling of processes occurring in sedimentary basins in geological time spans [4]. This includes deposition process modeling, pore pressure formation modeling, compaction and cementation simulation, determining paleo heat flow values (thermal history reconstruction), petroleum processes kinetics and eventually generation, expulsion, migration and accumulation formation simulation [4].

The process of model design proceeds in two stages: a geological model is defined – a model of rock parameters alteration during assumed structural evolution of basin, over geological time spans and thermal model is defined – a thermal evolution of the basin over geological time spans. A properly defined geological model is calibrated against porosity, permeability and pore pressure measurements. Thermal model is calibrated against thermal maturation indicators: vitrinite reflectance measurements or T_{max} values (obtained from Rock Eval pyrolysis) and against measured temperature in the borehole.

The basin model is divided into stages of it's structural evolution. Rock layers have assigned times of sedimentation – the model is divided into stages of deposition and erosion. Paleothickness of layers is reconstructed by back-stripping method [14]. At each time step, pore pressure formation is calculated in profile, because of the increasing weight of overburden layers – a result of newly deposited layers. Therefore, calculation of pressure and compaction is performed before thermal history reconstruction, at each time span.

Calibrated geological and thermal model is the basis for the calculation of processes within a defined petroleum system. Petroleum processes which took place in source rocks are key elements in modeling, because within them, shale gas deposits occurrence is expected.

As in the case of the classical approach a number of already generated hydrocarbons (expelled out of the source rock) is calculated. The most important element is to calculate the amount of hydrocarbons that had been generated, but didn't migrate out of the source rock.

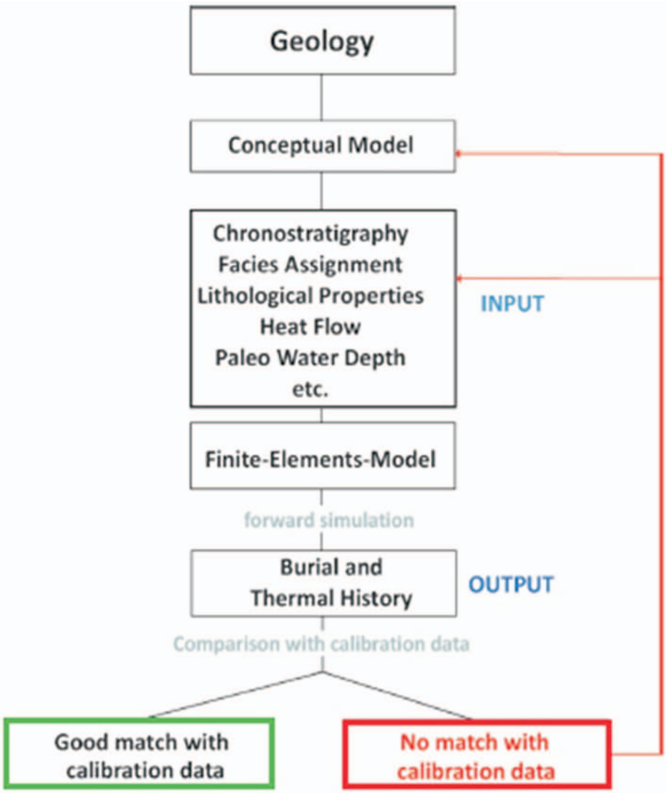


Fig. 1. Petroleum system modeling workflow [15]. After reaching a good match with calibration data, petroleum processes are calculated

Geology

Geological knowledge of the study area is crucial in order to determine the most important elements of basin evolution and their impact on thermal history of the basin, which have direct impact on the petroleum process.

The analyzed profile is located in the Baltic Syneclise which is located between the Baltic shield to the northwest and Mazurian-Belarusian Anteclise to the southeast. From the southwest the Baltic basin (Baltic Syneclise) is bordered by the Teisseyre – Tornquist Tectonic Zone which in Poland is considered to be the south-western edge of the Precambrian East European Craton and coincides with the north-eastern boundary of the Trans-European Suture Zone.

The geological structure of sedimentary cover is simple: rock layers usually lie almost horizontally. Paleozoic rocks lie directly on a crystalline basement.

The formation of the Baltic basin began in the late Neo-

proterozoic, and the main stage of its development occurred in the older Paleozoic. The Baltic basin was created as a result of the creation of a continental rift in the late Vend/Middle Cambrian [10].

After subsidence analysis it was concluded that after the Late-Proterozoic rifting stage – the western edge of the East European Craton was transformed into a passive margin shelf that during the middle (?) Ordovician/Silurian was subjected to flexural bending as a result of the collision of Avalonia and Baltica [9, 10]. At that time, the first source rocks had been formed.

In connection with the graben formation in the Upper Silurian foredeep, the accommodative area was where the largest and the highest rate of sedimentation were occurring. This event is recorded and represented as very thick Ludlovian and Pridoli layers. In Ludlovian layers debrits and turbitides appear as a sign of the presence of shale egzoflysh.

Upper Silurian sediments are the thickest part of whole Caledonian cover. In the early Devonian period significant structural reconstruction of the area was occurring which was accompanied by an intense uplift process – block tectonic movements. In the final stage of the Caledonian orogenesis the current structure of the Baltic basin was shaped. After that event a period of intense denudation appeared and sedimentation occurred, only locally [2].

Reconstruction of the extent of Devonian (Post-Devonian) erosion will be an important part of the modeling process. On the partially eroded Silurian layers lie Permian evaporates. Above them Alpine-aged sediments occur with total thickness of up to 800 m. In the studied area some of Mesozoic layers are not present. Lack of these layers could be related with paleoextent of the Jurassic and Cretaceous basins or with an erosion events. Small erosion events have been assumed in the model (Table 1). In the study area occur 200 m thick Cenozoic sediments.

Model construction and calibration

The first step of the basin model building is a definition of rock layers and time of their formation assignment. Specified lithological models are assigned to layers with their function in the petroleum system (Source Rock, Reservoir Rock, Seal Rock, Underburden, Overburden (Table 1). At this stage it is now possible to generate a burial plot of the analyzed borehole profile (Figure 2). Lithology models assigned to layers were selected based on available sedimentological, petrophysical and well log data. Lithology assignment is a very important step of modeling, because the properties of rocks should in the highest level reflect their actual measured parameters. Lithological models include these set of parameters: thermal conductivity, radiogenic heat, heat capacity, a model of mechanical compaction, permeability model (based on porosity values). The rock layer compaction model assigned to the lithology should simulate porosity decrease in geological time, with increasing overburden pressure (with burial) and in result it should predict measured porosity values. To define

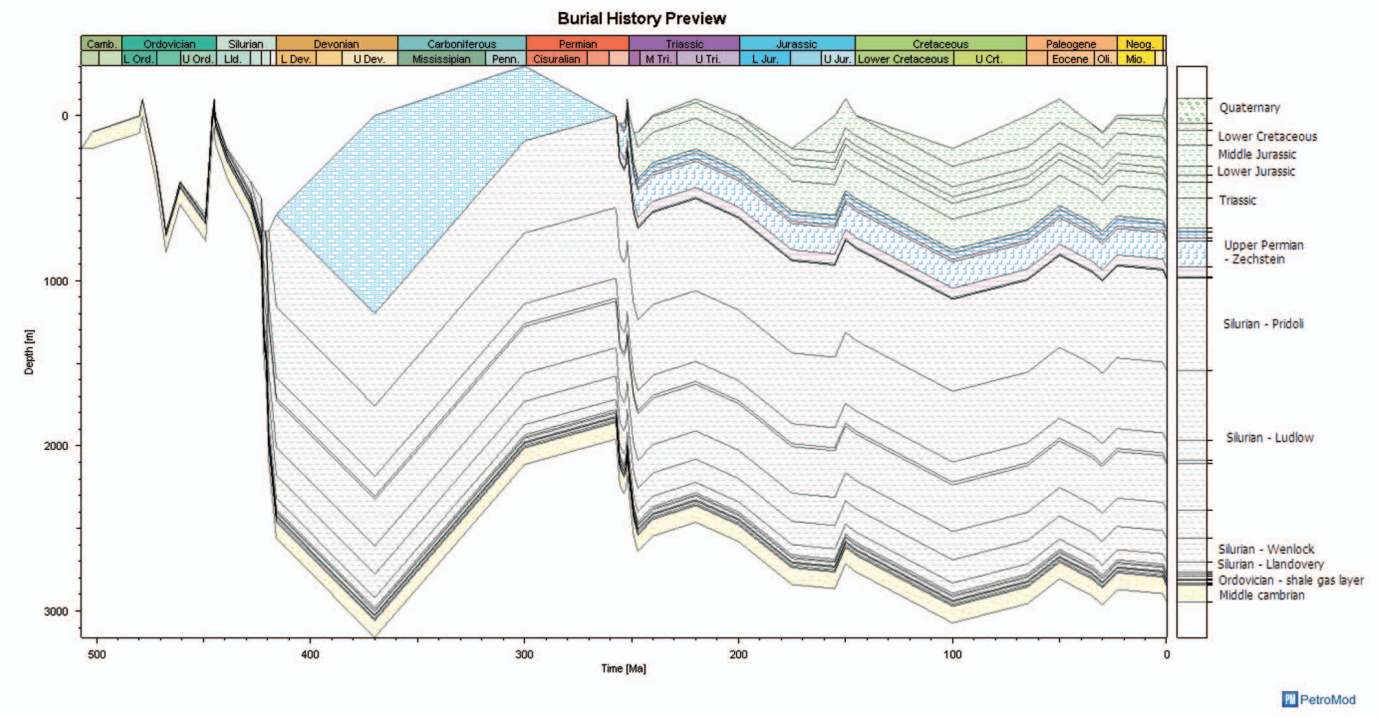


Fig. 2. Burial plot generated from Table 1

Table 1. Model inputs. Basin division into evolution stages with lithological models assignment and with petroleum system elements

Layer	Top [m]	Base [m]	Thickness [m]	Eroded [m]	Depo. Start [Ma]	Depo. End [Ma]	Erosion Start [Ma]	Erosion end [Ma]	Lithology	PSE
Quaternary	–106	49	155		1.80	0.00			Conglomerate (typical)	Overburden Rock
Tertiary	49	88	39		35.00	1.80			Siltstone (organic lean)_1	Overburden Rock
Lower Cretaceous	88	179	91	100	145.00	65.00	65.00	35.00	Siltstone (organic lean)_1	Overburden Rock
Middle Jurassic	179	304	125	100	175.00	155.00	155.00	145.00	Siltstone (organic lean)_1	Overburden Rock
Lower Jurassic	304	364	60		200.00	175.00			Siltstone (organic lean)_1	Overburden Rock
Triassic – Upper Pstry sandstone	364	404	40		247.00	200.00			Siltstone (organic lean)_1	Overburden Rock
Triassic – Middle Pstry sandstone	404	499	95		249.00	247.00			Siltstone (organic lean)_1	Overburden Rock
Triassic – Lower Pstry sandstone	499	683	184		252.00	249.00			Siltstone (organic lean)_1_1	Overburden Rock
Permian – Leine cyclotheme (Z3)	683	705	22		253.50	252.00			Dolomite (typical)	Seal Rock
Permian – Stassfurt cyclotheme (Z2)	705	743	38		255.00	253.50			Dolomite (typical)	Seal Rock
Permian – Upper Anhydrite (Z1)	743	758	15		255.50	255.00			Anhydrite	Seal Rock
Permian – Salt layers (Z1)	758	918	160		256.50	255.50			Salt	Seal Rock
Permian – Werra Anhydrite (Z1)	918	976	58		257.00	256.50			Anhydrite	Seal Rock
Permian – Zechstein (Z1)	976	984	8		257.50	257.00			Limestone (shaly)	Seal Rock
Devonian	984	984	0	1200	416.00	370.00	370.00	257.50	Limestone (shaly)	Reservoir Rock
Silurian – Pridoli	984	1542	558		419.50	416.00			Shale (typical)_1	Reservoir Rock
Silurian – Ludlow1	1542	1970	428		420.50	419.50			Shale (typical)_1	Reservoir Rock
Silurian – Ludlow2	1970	2091	121		421.00	420.50			Shale (typical)_1	Reservoir Rock
Silurian – Ludlow3	2091	2109	18		421.50	421.00			Shale (typical)_1	Reservoir Rock
Silurian – Ludlow4	2109	2391	282		422.50	421.50			Shale (typical)_1	Reservoir Rock
Silurian – Ludlow5	2391	2562	171		423.00	422.50			Shale (typical)_1	Reservoir Rock
Silurian – Wenlock	2562	2703	141		428.00	423.00			Shale (typical)_1	Reservoir Rock
Silurian – Llandovery1	2703	2765	62		439.00	428.00			Shale (typical)_1	Reservoir Rock
Silurian – Llandovery2	2765	2778	13		445.00	439.00			Shale (typical)_1	Source Rock
Ordovician – Aszgil	2778	2786	8		449.00	445.00			Shale (typical)_1	Seal Rock
Ordovician – Shale gas layer	2786	2806	20		461.00	449.00			Shale (black)_1	Source/Reservoir Rock
Ordovician – Lanwirn1	2806	2812	6		463.00	461.00			Shale (typical)_1	Reservoir Rock
Ordovician – Lanwirn2	2812	2815	3		467.50	463.00			Shale (typical)_1	Reservoir Rock
Ordovician – Arenigian1	2815	2829	14		472.00	467.50			Shale (typical)_1	Reservoir Rock
Ordovician – Arenigian2	2829	2838	9		477.00	472.00			Shale (typical)_1	Reservoir Rock
Upper Cambrian	2838	2844	6		502.00	480.00			Shale (typical)_1	Reservoir Rock
Middle Cambrian	2844	2944	100		507.00	502.00			Sandstone (clay rich)_1	Reservoir Rock

a suitable model for the compaction of each layer, decrease of porosity (started from initial porosity of sediment – obtained from experimental analysis) should be linked to pressure increase (or burial depth). Terzaghi type compaction models available in PetroMod software assume that the porosity of the sediment is formed when the rock is subject to the maximum effective pressure (at a maximum burial depth). Decompaction process which might have taken place in the analyzed area in the Devonian period during significant uplift – is neglected in the calculation.

The properly assigned compaction model should predict measured values of porosity. Well log data were used as calibration points (Figure 3). Petrophysical properties of rock layers also affect their thermal properties.

The first step in thermal model determination (paleotemperatures reconstruction in the basin) is boundary conditions assignment. For all specified time spans 3 values need to be assigned: HF – heat flow value (mW/m^2), SWI – Sediment-Water-Interface temperature (^{o}C), PWD – Paleo Water Depth (m) (Figure 4).

Paleo Water Depth values should be assigned based on sedimentary environments of rock layers formation. SWI parameter is calculated based on paleoclimate model and it is automatically calculated by software after inputting

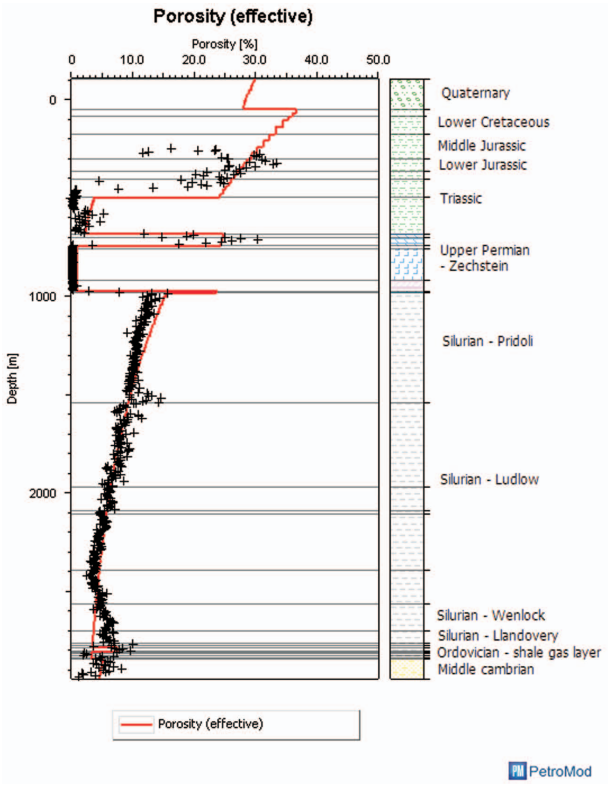


Fig. 3. Compaction model calibration in well profile. The black crosses are measured data, red line corresponds to calculated values from compaction models assigned for each rock layer

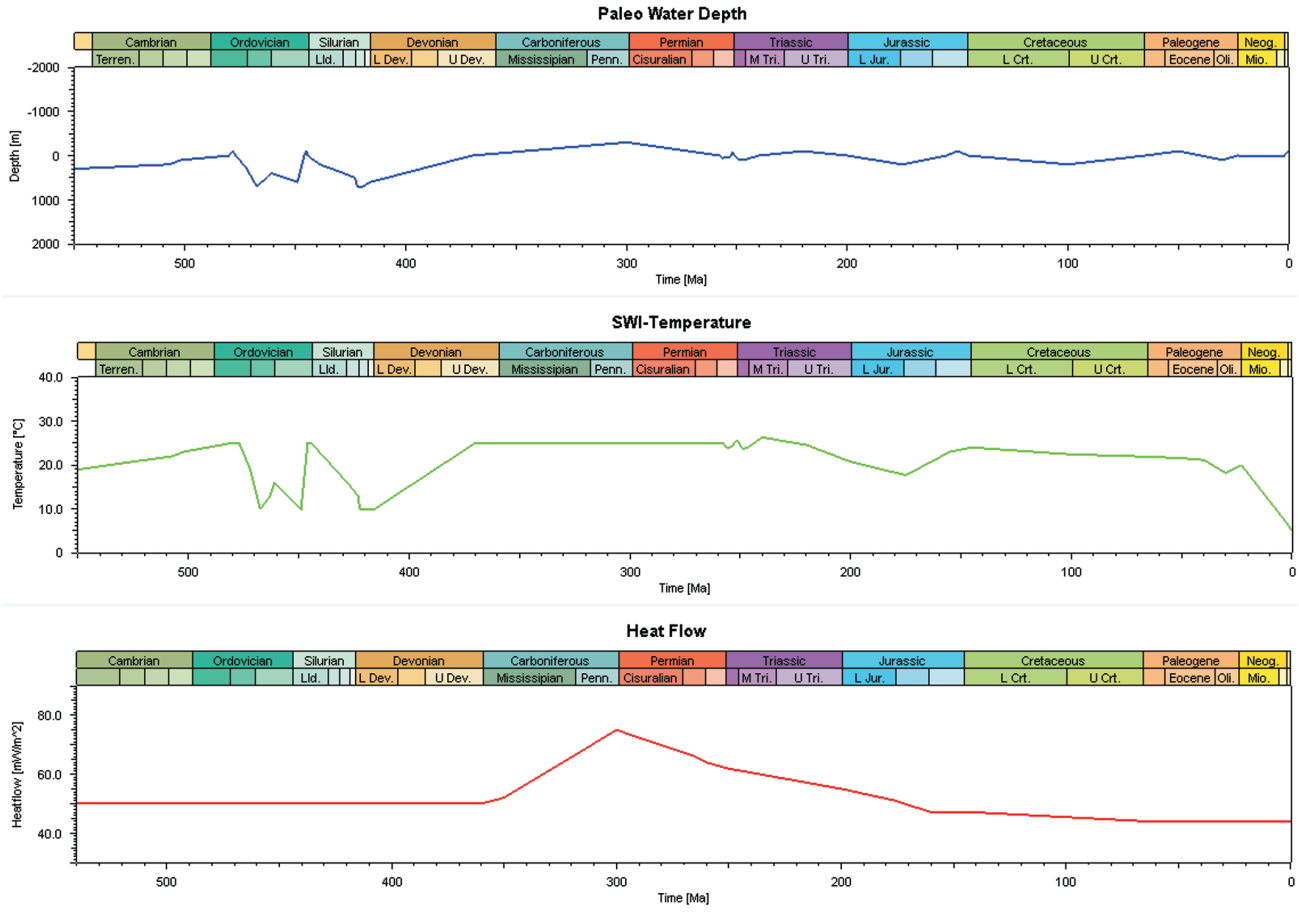


Fig. 4. Boundary conditions assigned in model

the latitude of the borehole position. At initial approach HF values were set as constant during all geological time spans and values were equal to present-day HF (calculated from borehole temperature) – 44 mW/m^2. Subsequently, thermal maturation is calculated based on assigned heat flow values. When increased values of HF between Carboniferous and Permian periods were assigned (due to widespread volcanic activity proven in this period) – calculated thermal maturity from the Sweeney & Burnham [11] model was close to measured values (Figure 5). Calculated present-day borehole temperature is also consistent with measured borehole temperature (Figure 6.)

When a satisfying match with calibration data is obtained – all models are assumed to be properly defined.

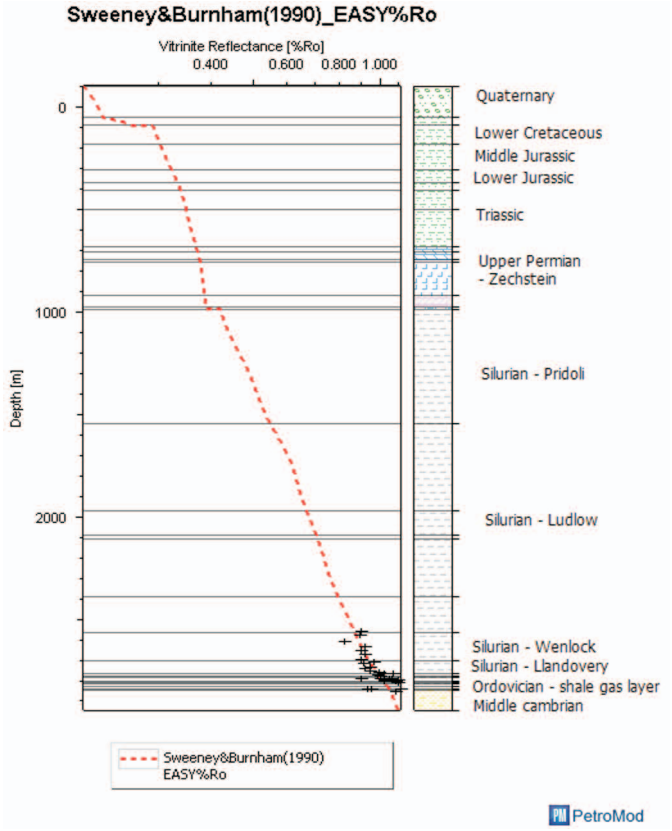


Fig. 5. Thermal model calibration in well profile. The black crosses are vitrinite reflectance values, red line represents calculated values from the Sweeney & Burnham [11] model

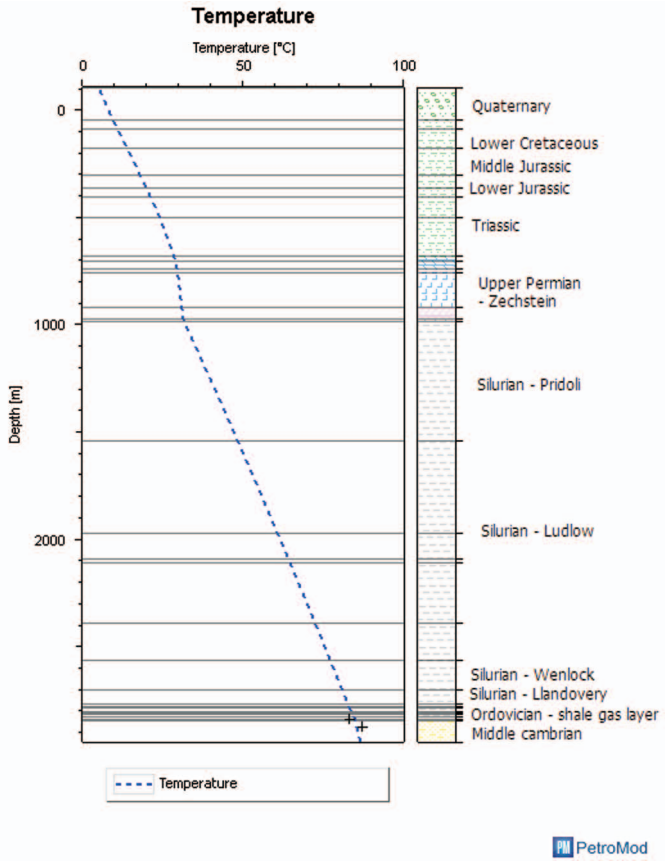


Fig. 6. Calculated present-day borehole temperature calibrated against measurements. The black cross is a measured value, blue line represents model values based on present-day heat flow

Hydrocarbon generation model

The main aim of 1D petroleum system modeling is the assessment of source rock hydrocarbon potential. For that purpose, hydrocarbon balance is performed: calculation of the quantity of already generated hydrocarbons during basin evolution. When it comes to unconventional plays assessment, calculation of generated and retained hydrocarbons (HC) within source rock is a key element. In order to determining the number of generated HC – source rock parameters need to be defined: initial TOC (%) content and initial Hydrogen Index (mg HC/g TOC) and kerogen kinetics based on kerogen type.

In this work all calculations concern the 20 meter thick Ordovician shale layer which is considered to be a source rock with shale gas potential. Based on Rock Eval measurements results, the kerogen type II kinetic model was assigned (with

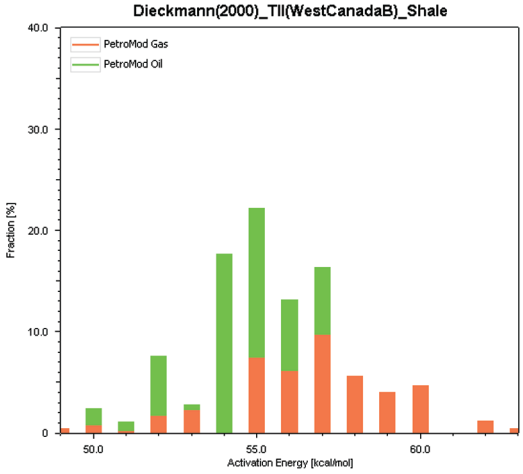
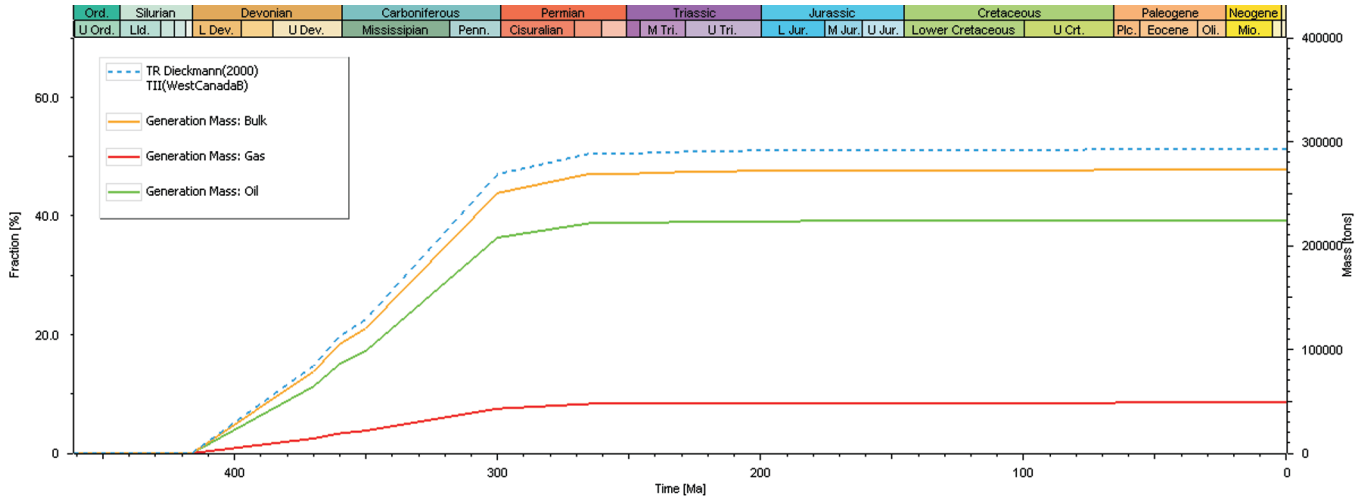


Fig. 7. Model of kerogen activation energy distribution with thermogenic products (oil and gas)

mixed oil and gas productivity) with specified activation energy distribution (Figure 7). Without defining the adsorption model, all generated hydrocarbons are considered to be expelled out of the source rock.



	Generation balance		Expulsion balance		Retention balance	
Mass [HC tons]	Oil	Gas	Oil	Gas	Oil	Gas
Ordovician shale gas layer	224203.59	48672.22	224203.59	48672.22	0	0

Fig. 8. Hydrocarbon balance for Ordovician source rock cell 20 × 1000 × 1000 m. The blue line refers to kerogen transformation ratio calculated from kerogen kinetics

Hydrocarbons retention/adsorption model

In order to calculate the number of hydrocarbons which are present within the source rock – the adsorption model should be incorporated based on available sorption capacity measurements. It turns out that Total Gas values obtained from laboratory measurements of cores are almost similar to sorption capacity measurements, and that was the base for the assumption that almost 100% of measured gas is sorbed within kerogen. Additionally, significant correlation of sorption capacity (Langmuir volume) with total organic carbon was found (Figure 9).

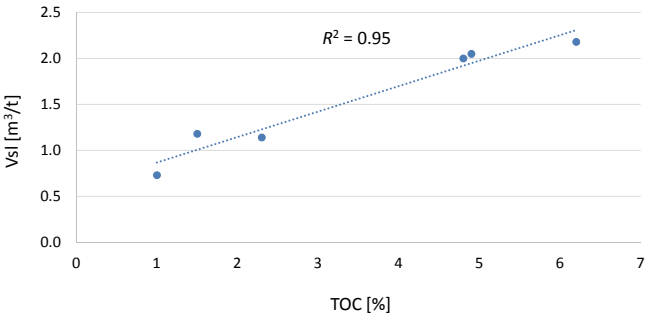


Fig. 9. Sorption capacity vs. total organic carbon content (commissioned works ordered by the Oil and Gas Institute – NRI)

PetroMod software has the ability to integrate the Langmuir adsorption model for gas. Five parameters need to be used as input: Langmuir volume (maximum volume of gas adsorbed by sample/weight of sample), Langmuir pressure and temperature (pressure and temperature at which measurement has been conducted), measured TOC, desorption energy (energy required to desorb already adsorbed hydrocarbons when rock undergoes different pressure-temperature regime – this value was defined based on Gasparik papers [3] (Figure 10).

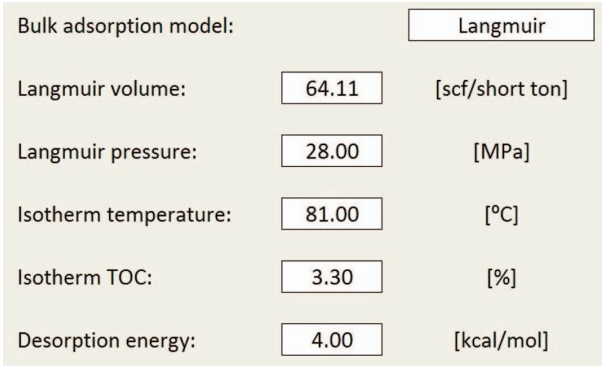
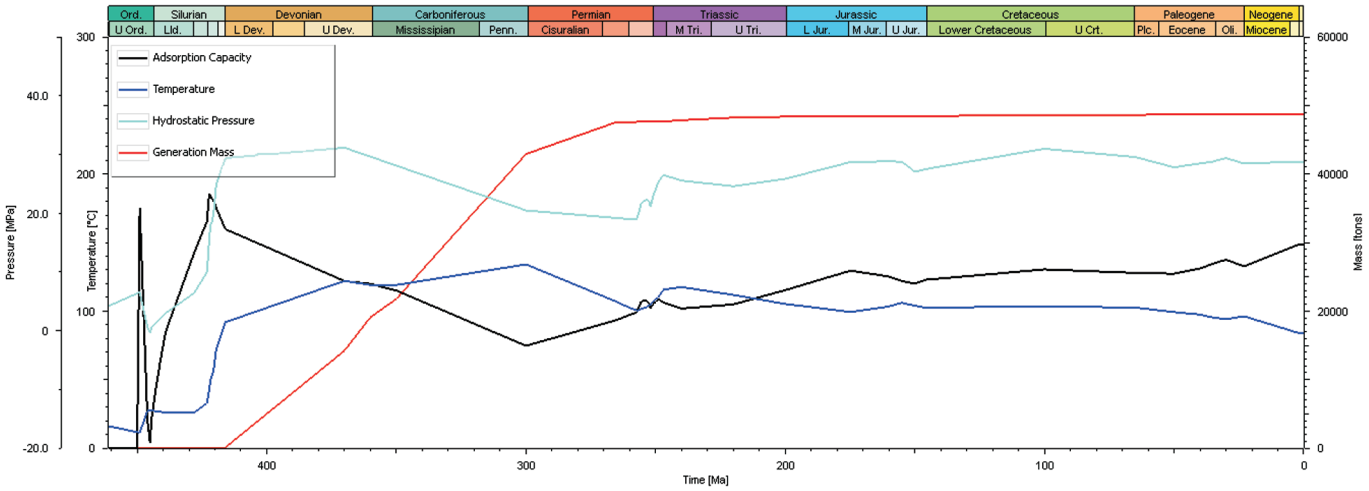


Fig. 10. Langmuir adsorption model for gas – input parameters

Calculated Ordovician source rock adsorption capacity for gaseous hydrocarbons was 0.83 m^3/t rock. 61% of generated gaseous hydrocarbons were retained within the Ordovician source rock. 39% of gaseous hydrocarbons were expelled out of the rock. This model is applicable only for gas retention (adsorption) calculation (Figure 11).

In order to calculate the amount of retained liquid hydrocarbons within source rock, simple calculation was applied.



	Generation balance		Expulsion balance		Retention balance	
Mass [HC tons]	Oil	Gas	Oil	Gas	Oil	Gas
Ordovician shale gas layer	224203.59	48672.22	224203.59	18924.44	0	29747.78

Fig. 11. Gas generation balance for Ordovician source rock cell 20 × 1000 × 1000 [m] with Langmuir adsorption model. Influence of pressure and temperature on adsorption capacity is shown

For this purpose the Rock Eval parameter was used: S1 (mg HC/g rock) which refers to the number of liquid hydrocarbons which occur within a source rock. The average S1 content in the analyzed interval is 2.05 mg HC/g of rock. This parameter is well correlated with extractable organic matter (Figure 12).

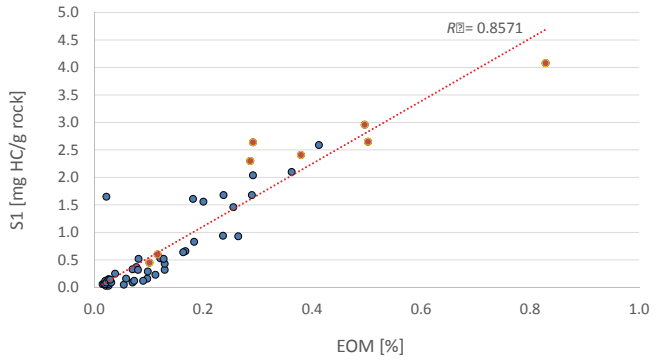


Fig. 12. Liquid hydrocarbon content from Rock Eval pyrolysis vs. extracable organic matter from laboratory measurements. The orange points come from the Ordovician layer (Oil and Gas Institute works – NRI)

There is an indication that these hydrocarbons have syngenetic origins – so they were formed in-situ as a result of generation processes and have been preserved within the rock, either in the adsorbed form or in free form in the pore space of the rock (Figure 13). For good hydrocarbon balance calculation, the form of hydrocarbons retention within a source rock is not important.

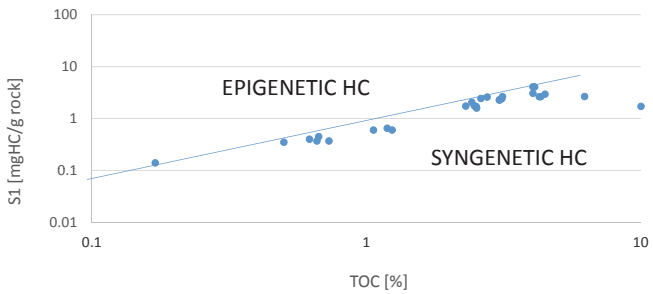
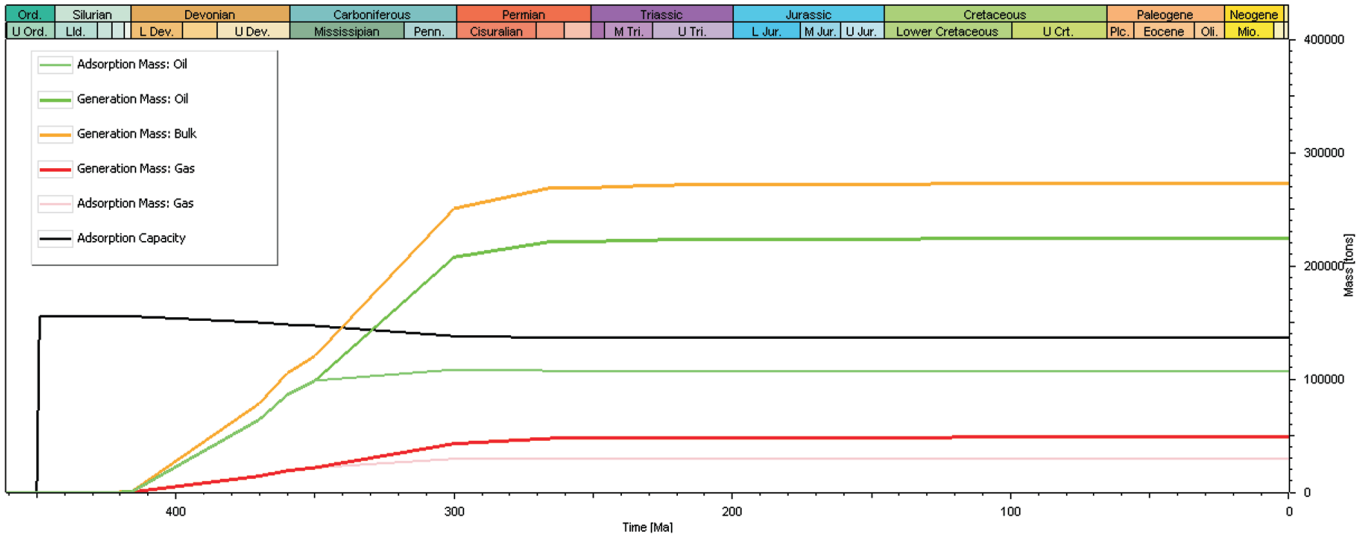


Fig. 13. Genetic characterization of liquid hydrocarbons which occur within source rock (Oil and Gas Institute – NRI works)

During the modeling of the retention of liquid and gaseous hydrocarbons within source rock, simple model of kerogen sorption capacity was used. Having a coefficient of 0.015 for kerogen sorption capacity for gaseous hydrocarbons and 0.055 for liquid hydrocarbons, an amount of gaseous and liquid hydrocarbons corresponding to that obtained from the measurements sorption capacity and Rock Eval measurements. Application of different hydrocarbon retention models don't affect the already calculated quantity of generated hydrocarbons.

The calculated total amount of retained hydrocarbons (present in the adsorbed phase and free form in the source rock) relative to the amount of hydrocarbons already generated is around 50%. This result is significantly higher than those previously calculated in these types of models [1, 12]. In the context of the petroleum system model this simplified approach has a great impact on hydrocarbon balance calculation (Figure 14).



	Generation balance		Expulsion balance		Retention balance	
Mass [HC tons]	Oil	Gas	Oil	Gas	Oil	Gas
Ordovician shale gas layer	224203.59	48672.22	117076.4	18924.44	107127.2	29747.78

Fig. 14. Calculated hydrocarbon balance for Ordovician shale source rock cell 20 ×1000 × 1000 [m] with simple adsorption model for gaseous and liquid hydrocarbons

Summary and conclusions

1. The modeling approach shown in this paper is based on very simple assumptions, nevertheless it shows the great importance of the role of inputting the number of retained hydrocarbons in hydrocarbon balance.
2. It is possible to apply Langmuir gas adsorption model in petroleum system modeling and therefore to calculate source rock sorption capacity, depending on the pressure and temperature. This model can be used only in the case of the hydrocarbon balance of gaseous hydrocarbons.
3. The kerogen sorption model of gaseous and liquid hydrocarbons has no ability to distinguish the retention processes (adsorbed or free form) – it is a simple model which depends only on the amount of organic carbon in the layer which is an adsorbent and does not depend on the pressure and temperature.
4. The calculated quantity of hydrocarbons retained in the analyzed Ordovician shale layer is around 50% of the total generated hydrocarbons from this unit. Without taking into account the retention process, this amount of hydrocarbons will be calculated as expelled out of the source rocks and could lead to overestimation of potential hydrocarbons which could form conventional reservoirs within the petroleum system.
5. In order to properly determine the level of liquid hydrocarbons which were generated in-situ in the Ordovician source rock, their epigenetic origins should be excluded by additional analysis (biomarkers, the isotopic composition of gas).
6. For reliable hydrocarbon generation process reconstruction, experimental studies should be carried out for determining the actual kinetic parameters of kerogen.

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