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# A COMPARATIVE ANALYSIS OF DIFFERENT KINETIC MODELS FOR CALCULATING VITRINITE REFLECTANCE IN SOURCE ROCKS FOR OIL AND GAS IN THE BANAT DEPRESSION (SERBIA)

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**Abstract**

This paper presents, for the first time, the application of the Vitrinite Math software program for assessing the thermal maturity of organic matter through vitrinite reflectance modelling (Ro). The calculations were performed using five different kinetic models: Easy%Ro, Press%Ro, IKU%Ro, T-P-Ro, and Basin%Ro. Although laboratory-measured vitrinite reflectance values are essential for determining the maturity stage of organic matter, their comparative analysis using multiple kinetic models enhances the accuracy and reliability of interpreting results on the thermal maturity of organic matter, which is a crucial aspect of petroleum-geological research. Multiple modelling reduces the risk of erroneous conclusions when assessing the generative potential of source rocks, especially in complex sedimentary systems when exploring oil and gas deposits. The results presented in the paper indicate that the kinetic models Press%Ro and T-P-Ro, which include overpressures, show the best agreement with the measured down to 3490 m, while among the kinetic models that do not include overpressure, Basin%Ro exhibits a high correlation with the measured %Ro values.

**Key words:** vitrinite math, kinetic models, vitrinite reflectance, thermal maturity, source rocks

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**Introduction.** The vitrinite reflectance method refers to reflection photometry used to determine the maturity level of organic matter dispersed in sediments or accumulated in coals. Vitrinite reflectance (%Ro) is based on measuring the reflected incident light from the polished surface of vitrinite particles (referred to as 'huminite' in diagenesis). Reflectance measurements are performed under a microscope in immersion oil with a refractive index of 1.518 at a wavelength of 546 nm [1]. The mean random reflection (%Ro), which is most commonly used today and corresponds to the oil window, varies depending on the type of organic matter and the heating rate [2]. The usual vitrinite reflectance values associated with start of oil generation from kerogen are around 0.50% Ro, while the value of 0.60% Ro is widely accepted as the maturity level necessary to generate and release sufficient quantities of hydrocarbons for accumulation in commercial deposits [3].

The paper presents, for the first time, the results of the Vitrinite Math software program, which is used to calculate vitrinite reflectance based on input parameters. The given calculation was performed using five different kinetic models: Easy%Ro, Press%Ro, IKU%Ro, T-P-Ro, and Basin%Ro, based on data from the southeastern part of the Pannonian Basin in Serbia, specifically from the Banat Depression area. Although laboratory data of vitrinite reflectance form the basis for assessing thermal maturity, their verification through multiple kinetic models enables a more accurate calibration of geological and thermal models. This approach reduces the risk of misinterpreting the conditions of thermal maturation of organic matter in a sedimentary basin and enables a reliable assessment of the generative potential of the analyzed source rocks. Figure 1 shows the structural map of the Banat Depression together with the A–A′ backstripping profile [3].

**Samples and methods.** The measured vitrinite reflectance values of 31 source rock samples for oil and gas from the Banat Depression in the northern part of Serbia, taken at depths ranging from 1410 m to 3490 m, were used to correlate the kinetic model calculations in the Vitrinite Math program. The geological structure of the studied part of the Banat Depression includes Badenian, Sarmatian, Pannonian, Pontian, Pliocene, and Quaternary sediments. The source rocks, according to their lithological composition, are presented by marls with sandstone interbeds, clays, limestones and very rarely, black shales containing traces of oil in fractures, dating from the Badenian, Sarmatian, Pannonian, and Pontian ages. Based on previous geochemical analyses, the Pannonian sediments in particular indicate good effective source rocks for oil and gas in this area, as they are characterized by a favourable kerogen type and abundance, significant total organic carbon (TOC) contents, and a good remaining generative potential (S2), being within the main oil-generation window [4]. The average vitrinite reflectance values of the analyzed samples range from 0.41% Ro at a depth of 1410 m to 0.86% Ro at a depth of 3490 m. Considering the results of the measured vitrinite reflectance, it is observed that the increase in reflectance correlates with the increase in depth. According to the available data, vitrinite reflectance values above 0.50%

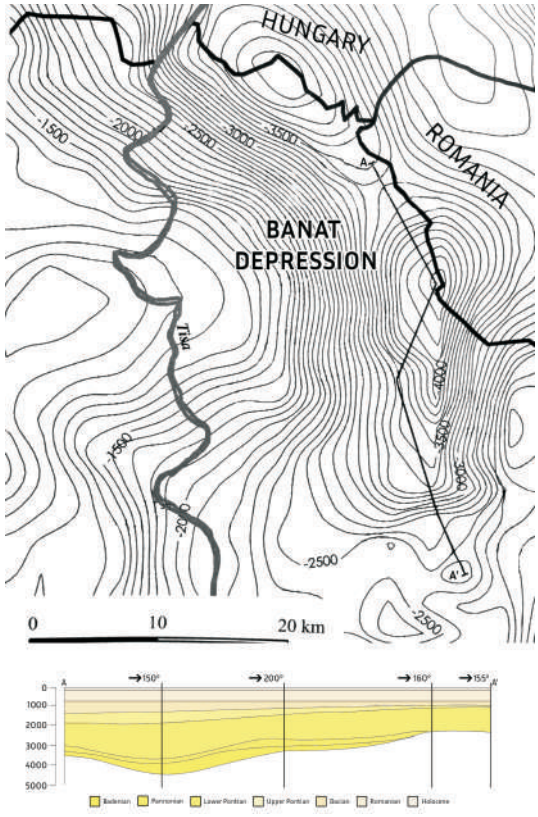



Fig. 1. Structural map of the Banat Depression and A–A′ backstripping profile, modified from [3]

Ro correspond to sediments at approximately 120 °C; a reflectance of 0.60% Ro corresponds to a temperature of 140 °C, while at 170 °C, the reflectance is around 0.80% Ro. At temperatures above 175 °C, there is generally a sharp increase in vitrinite reflectance, reaching a value of around 1.00% Ro near 180 °C [4].

The kinetic models Easy%Ro, Press%Ro, IKU%Ro, T-P-Ro, and Basin%Ro were selected for application in the Vitrinite Math software because together they represent the main approaches to thermal maturity assessment. Easy%Ro serves as the fundamental historical model, whereas IKU%Ro provides a fundamental pressure-independent alternative formulation. Press%Ro and T-P-Ro account for pressure effects and variations in kinetic structures, while Basin%Ro provides an independent approach by applying different stoichiometric coefficients and a distinct relationship between transformation ratio and vitrinite reflectance, thereby enabling direct comparison of different kinetic assumptions.

The task of the Vitrinite Math software program is to calculate vitrinite reflectance at given depths based on input parameters and to present the results as clearly and reliably as possible, applying the fundamental principles of organic

matter thermal maturation and hydrocarbon generation [5]. Depending on the model used, the input parameters may vary. The Easy%Ro model is the most commonly used kinetic model for assessing the maturity of organic matter [6]. It uses activation energies in the range of E = 34–72 kcal/mol, while the Arrhenius frequency factor is $A = 1 \times 10^{13}$/s. The model is characterized by its exceptional performance across a wide range of heating rates, from those under laboratory conditions – such as 1 °C per week – to those found in real geological settings [7]. The Easy%Ro model accounts for the effects of time and temperature without direct dependence on pressure [6]. The IKU%Ro model uses a more complex distribution of activation energies, which provides a better description of type II and III kerogens and covers a wider temperature range compared to the Easy%Ro model [8]. It was developed by the Norwegian Institute for Continental Shelf Research (IKU). The Basin%Ro kinetic model is a complex model that takes into account not only temperature and time, but also fluid migration and changes in pore pressures over geological time. It incorporates the influence of a multiphase system with variations in porosity and permeability. This model is particularly useful for a more accurate assessment of the thermal maturity of organic matter compared to traditional models such as Easy%Ro [9]. The Press%Ro model incorporates the effects of overpressure and its influence on the thermal evolution of organic matter [10], while the T-P-Ro kinetic model also uses Arrhenius kinetics but modifies the activation energy and frequency factors to account for the impact of pressure. Its significance lies particularly in assessing the maturity level of organic matter and oil generation, as high pressures can shift the start and end of the oil window to greater depths [11].

For the kinetic models Easy%Ro, IKU%Ro, and Basin%Ro, the input parameters used were age and temperature, while for Press%Ro and T-P-Ro, overpressure was also included as an input parameter. It is important to note that if overpressure is not present in the basin, or if no value for it is entered, the models that use it as an input parameter will produce the same results as Easy%Ro. For this reason, the program allows the option to disable the input of overpressure, in which case Press%Ro and T-P-Ro will not be calculated.

After entering all relevant data into the appropriate tables within the Vitrinite Math software program, activating the 'Calculate' option triggers the automatic computation and filling in of the columns related to the kinetic models (Table 1). For easier visual interpretation of the thermal maturity of organic matter, the obtained values are colour-coded according to the level of vitrinite reflectance (Ro), which is a standard indicator of the thermal maturity of organic matter in sedimentary basins. Graphs can be created for each kinetic model individually, as well as for their combinations, which contributes to a more detailed comparison of results and better correlation among the kinetic models. If measured vitrinite reflectance values are available, they may also be displayed on the graphs, as shown in the paper. This allows for a comparison between modelled and actual

Table 1

Input parameters with calculated reflectance values

| # | Time | Depth | Temp | Over-pressure | Easy%Ro | Press%Ro | IKU%Ro | T-P-Ro | Basin%Ro |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.00 | 300.00 | 25.25 | 0.00 | 0.24 | 0.24 | 0.21 | 0.24 | 0.23 |
| 2 | 3.80 | 1300.00 | 72.25 | 0.00 | 0.35 | 0.35 | 0.29 | 0.35 | 0.36 |
| 3 | 5.30 | 1600.00 | 87.00 | 0.00 | 0.43 | 0.43 | 0.36 | 0.43 | 0.44 |
| 4 | 7.30 | 2200.00 | 115.50 | 29.60 | 0.60 | 0.58 | 0.49 | 0.58 | 0.54 |
| 5 | 9.00 | 4150.00 | 208.13 | 318.40 | 1.67 | 0.92 | 1.74 | 1.05 | 1.61 |
| 6 | 11.60 | 4400.00 | 220.00 | 355.40 | 2.42 | 1.25 | 3.75 | 1.47 | 2.94 |
| 7 | 13.00 | 4450.00 | 222.38 | 362.90 | 2.60 | 1.33 | 4.09 | 1.57 | 3.26 |
| 8 | 14.00 | 4650.00 | 231.88 | 392.40 | 2.74 | 1.38 | 4.34 | 1.65 | 3.49 |

measured data, which is particularly important for validating geothermal models and assessing the generative potential of source rocks for oil and gas.

**Results.** For the input parameters in the Vitrinite Math program, eight data points with known ages, depths, and overpressure values were used, as shown in Table 1. The units presented in the table are Ma for age (time), meters (m) for depth, degrees Celsius (°C) for temperature, and bar for overpressure. The geothermal gradient used was 47.5 °C/km, and the surface temperature was 11 °C. Due to the low resolution of the input data, especially within the depth range containing measured values, the data were interpolated by depth. The total number of data points after interpolation is one thousand, which significantly increases the resolution and accuracy of the results. In addition to depth interpolation, as shown in the paper, the program also offers the option of interpolation by age. The tables presented in the paper were taken directly from the PDF report generated by the Vitrinite Math program.

Table 1 summarizes the calculated vitrinite reflectance (%Ro) values derived from various kinetic models as functions of depth, temperature, and pressure. In this study, the analysis is confined to depths up to 3490 m, as measured vitrinite reflectance data are available only to this depth, ensuring a reliable evaluation of the model predictions. Within the table, this corresponds to depths of approximately 2200 m.

At depths ranging from 300 to 1600 m, under temperatures of approximately 25–87 °C and in the absence of overpressure, the calculated vitrinite reflectance values range between 0.21 and 0.44 %Ro. The Easy%Ro model yields slightly higher values (0.24–0.43% Ro) compared to IKU%Ro (0.21–0.36% Ro) and Basin%Ro (0.23–0.44% Ro), while Press%Ro and T-P-Ro produce values practically identical to Easy%Ro within this interval. All results indicate an immature

to early stage of thermal maturity. At a depth of 2200 m, under a temperature of 115.5 °C, where the onset of moderate overpressure (∼30 bar) is observed, differentiation among the applied kinetic models becomes apparent. The Easy%Ro model provides the highest calculated vitrinite reflectance values of 0.60% Ro. Models that explicitly account for pressure, Press%Ro and T-P-Ro, yield nearly identical values of 0.58% Ro, slightly lower than the maximum values predicted by Easy%Ro. The Basin%Ro model gives intermediate reflectance values, approximately 0.54% Ro, whereas IKU%Ro shows the lowest calculated values of 0.49% Ro. The values for depths below 3490 m, and particularly for depths greater than 4000 m, are based on model assumptions and were not analyzed in detail in this study, with only their representation provided.

Figure 2 presents two graphs generated using the input parameters in the Vitrinite Math software program, showing comparative vitrinite reflectance values. On both graphs, the white circles indicate the measured vitrinite reflectance values for a total of 31 samples from the Banat Depression down to a depth of 3490 m.

The analysis of the given graphs reveals that the Easy%Ro model shows the greatest deviations from the measured values, while the other models exhibit significantly better agreement. Given that the software includes both the directly measured vitrinite reflectance data and the parameters for reflectance calculation, it is possible to calculate the average absolute and relative error for each of the applied models. In the case of the Banat Depression, the most reliable results were obtained from the models that use overpressure as an input parameter. Among them, the T-P-Ro model (relative error = 5.88%) shows the best agreement with the measured data, with an average deviation of only 0.17% lower compared to the Press%Ro model (relative error 6.05%). Next in terms of accuracy is the Basin%Ro model (relative error = 7.36%), whose results – although they omit overpressure in the calculation – show a high correlation with the measured values. The IKU%Ro model exhibits a relative error of 11.77%, whereas the Easy%Ro model is characterized by the highest relative error of 12.25%.

The Basin%Ro and IKU%Ro models show very similar shapes of the reflectance curves (Fig. 2), characterized by two linear segments. The first segment, up to approximately 0.75% Ro, is marked by a gradual increase in reflectance, followed by a sharp rise. The difference between these two models lies in the nature of the transition between the two segments – in the case of IKU%Ro, the transition is significantly more gradual, but it is precisely in this interval that the model shows a distinct deviation from the measured vitrinite reflectance values in the Banat Depression domain. As a consequence, the total error for the IKU%Ro model is significantly closer to that of the Easy%Ro model than to the Basin%Ro model. Based on the presented results, it can be concluded that the Easy%Ro and IKU%Ro models have not proven to be reliable under the conditions of the Banat Depression, given the relative errors exceeding 10%.

In addition to all aforementioned results, the Vitrinite Math software program

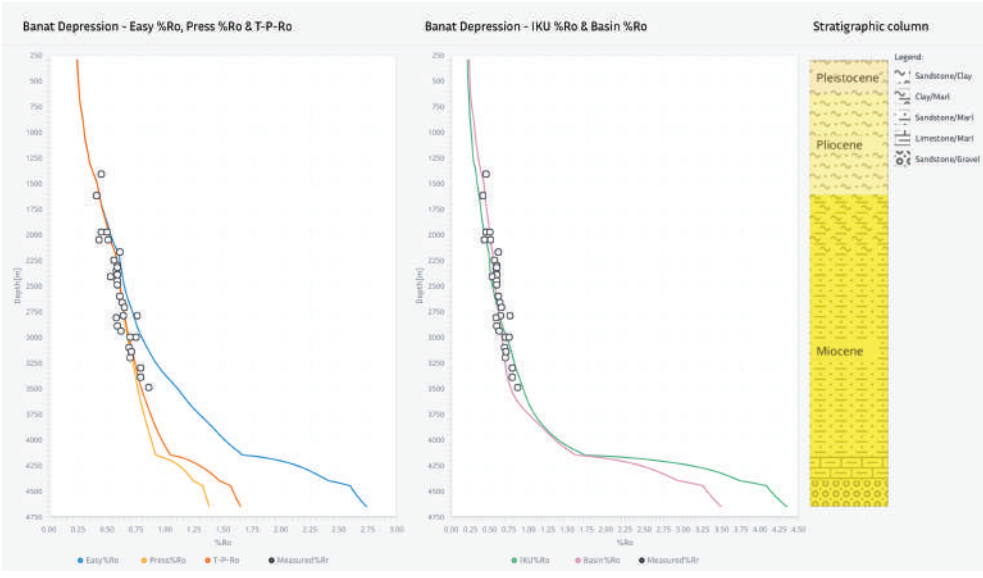



Fig. 2. Graphic representation of the kinetic models Easy%Ro, Press%Ro and T-P-Ro (left) and IKU%Ro and Basin%Ro (right) in the area of the Banat Depression with a stratigraphic column

also calculates estimates of the depths of the oil and gas window boundaries. By interpolating the nearest input parameters relative to the boundary values (0.50% Ro, 0.80% Ro, and 1.1% Ro), the depths for the start of the oil and gas windows, as well as the end of the oil window, are obtained according to each model (Table 2).

T a b l e 2

Estimated depths of the oil and gas window boundaries

| Estimated boundaries of oil and gas window | | | |
|---|---|---|---|
| Model | Oil window start (km) | Gas window start (km) | Oil window end (km) |
| Easy%Ro | 1.88 | 3.00 | 3.49 |
| Press%Ro | 1.91 | 3.67 | 4.23 |
| IKU%Ro | 2.31 | 3.20 | 3.77 |
| T-P-Ro | 1.91 | 3.51 | 4.16 |
| Basin%Ro | 2.00 | 3.55 | 3.82 |

Analysis of Table 2 shows that the IKU%Ro model predicts a significantly deeper onset of the oil window compared to the other models, up to 310 m deeper than the next deepest, Basin%Ro, due to lower reflectance values at lower temperatures. However, owing to the rapid increase in reflectance with temperature, the gas window onset and oil window end predicted by IKU%Ro are much closer to those of the other models. Models incorporating overpressure (Press%Ro and

T-P-Ro) yield results similar to Easy%Ro at shallower depths, but with increasing overpressure, the differences become more pronounced, resulting in the deepest predicted oil window terminations. Press%Ro exhibits a stronger overpressure effect compared to T-P-Ro. Easy%Ro predicts the shallowest maturity boundaries, associated with overestimated reflectance values, whereas measured boundary reflectances are closest to the depths predicted by the Basin%Ro model.

**Conclusion.** A comparative analysis of different kinetic models for calculating vitrinite reflectance in the Banat Depression with measured values down to a depth of 3490 m, shows that models incorporating overpressure (T-P-Ro and Press%Ro) provide the most accurate estimates of thermal maturity and the delineation of the oil window boundaries. Models without overpressure (Easy%Ro and IKU%Ro) display higher %Ro values in shallow layers and delay the onset of the oil window, resulting in greater deviations compared to measured %Ro values. The Basin%Ro kinetic model, although not accounting for overpressure, achieves a high correlation with measured %Ro values and represents a reliable estimate of source rock thermal maturity. Based on the obtained results, it can be concluded that the Vitrinite Math software program, which enables the calculation of vitrinite reflectance using various kinetic models, represents a reliable and efficient tool for assessing the thermal maturity of organic matter, as well as the generative potential of source rocks for oil and gas. Accordingly, the Vitrinite Math program, the application of which is presented for the first time in this paper, can play an important role in modern approaches to regional oil and gas deposit exploration.

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