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Thermal Maturation Trend and Cluster Validation Using K-Means Clustering: Case Study in Salawati Basin

Arista Muhartanto[1], Yarra Sutadiwiria[1], Mordekhai[2], Imam Setiaji Ronoatmojo[1], [1]Cahyaningratri Prima Riyandhani[1], and Burhannudinnur[1]

[1]Geology Department, Faculty of Earth Technology and Energy, Universitas Trisakti, Jalan Kyai Tapa No. 1, Jakarta 11440, Indonesia
[2]Geovartha, Jl. Dr. Nurdin 1 No.21, Jakarta 11450, Indonesia

Corresponding author: yarra.sutadiwiria@trisakti.ac.id
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Abstract - In the last few years, exploration activities have experienced obstacles and have not attracted much attention from researchers in Indonesia. One of the basins in Indonesia that is still interesting is Salawati Basin in West Papua, Indonesia. Several studies related to petroleum systems have been carried out in this basin, especially those that control the migration of hydrocarbon in Salawati Basin. This research was conducted on three wells located in the western of Salawati Basin to evaluate the characteristics and the maturity of the source rock, especially the Sirga Formation. This formation is penetrated by wells MM-02, MM-03, and MM-04, by using the K-Means Clustering method to validate several parameter variations of the maturity level. K-means cluster performs data from various parameters of maturity level with predefined three numbers of cluster. The thermal evolution of source rocks can alter organic matter physical and chemical properties, converting it into hydrocarbon compounds. The selected maturity parameters have good sensitivity to the determination of thermal maturity including phenanthrene (P), in addition to the MPI (methylphenanthrene index) parameter which was obtained from mass chromatograms m/z 178 and m/z 192 based on the peak area of P and methylphenanthrene (MP). Based on the appearance of the crossplot, both Radke and Kvalheim Formulas show that the maturity in studied area is divided into three main zones: peak maturity zone, early maturity zone, and outliers. This study also found that increasing thermal maturity is correlative with the increasing depth.

Keywords: Salawati Basin; methylphenanthrene index; K-means clustering; maturity

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Introduction

Background

One of the efforts to meet Indonesia growing energy needs is to increase exploration activities, especially in areas that still have hydrocarbon potential. In the last few years, exploration activities have experienced obstacles and have not attracted much attention to researchers in Indonesia, especially in eastern Indonesia. An area in eastern Indonesia that still attracts the attention of researchers is Salawati Basin in West Papua.

Salawati Basin is a large enough hydrocarbon-producing basin with the presence of hydrocarbon exploration activities.

Several studies related to petroleum systems have been carried out in this basin, especially those that control the migration of hydrocarbon in Salawati Basin. The geochemical studies which state that Middle Miocene claystone from Klasafet Formation with claystone and shale from Klasaman Formation are the source rocks that produce oil in Salawati Basin, in addition to the limestone of Kais Formation which is also assumed to be an Early Miocene source rock (Pireno and Noeradi, 2014). The Klasafet Formation is assumed to be ineffective in the formation of hydrocarbon, because it is still in the early mature phase. This can be seen in several models of hydrocarbon maturation from several locations in Salawati Basin (Pireno and Noeradi, 2014). Both researchers also deliver that the discovery of oil in pre-Kais sandstones in 2008 could become new supporting evidence that Sirga Formation is assumed to be an oil source-rock in Salawati Basin trapped within the lower (intra-Kais) limestone of the Kais Formation.

The application of biomarkers to determine the maturity of sedimentary and oil samples is focused on parameters based on sterane, triterpane, and aromatics. After the oil formation stage enters the gas window, the biomarkers of n-alkanes and triterpanes (aliphatic hydrocarbon) are no longer reliable as indicators of maturity. Therefore, after the final stage of oil formation, the parameters of aromatic hydrocarbons are used. Aromatic hydrocarbon indicators based on trimethylnaphthalenes (TNR), methylphenanthrenes (MP), and dimethylnaphthalenes (DNR) are considered the most reliable. Developing a thermal maturity formula based on MP parameters was the aim of this study (Radke and Welte, 1983), with expectations to have their own novelty value from this study. This study was conducted on three wells located in the western of Salawati Basin (Figure 1) to evaluate the characteristics and the maturity of the source rock, especially the Sirga Formation.

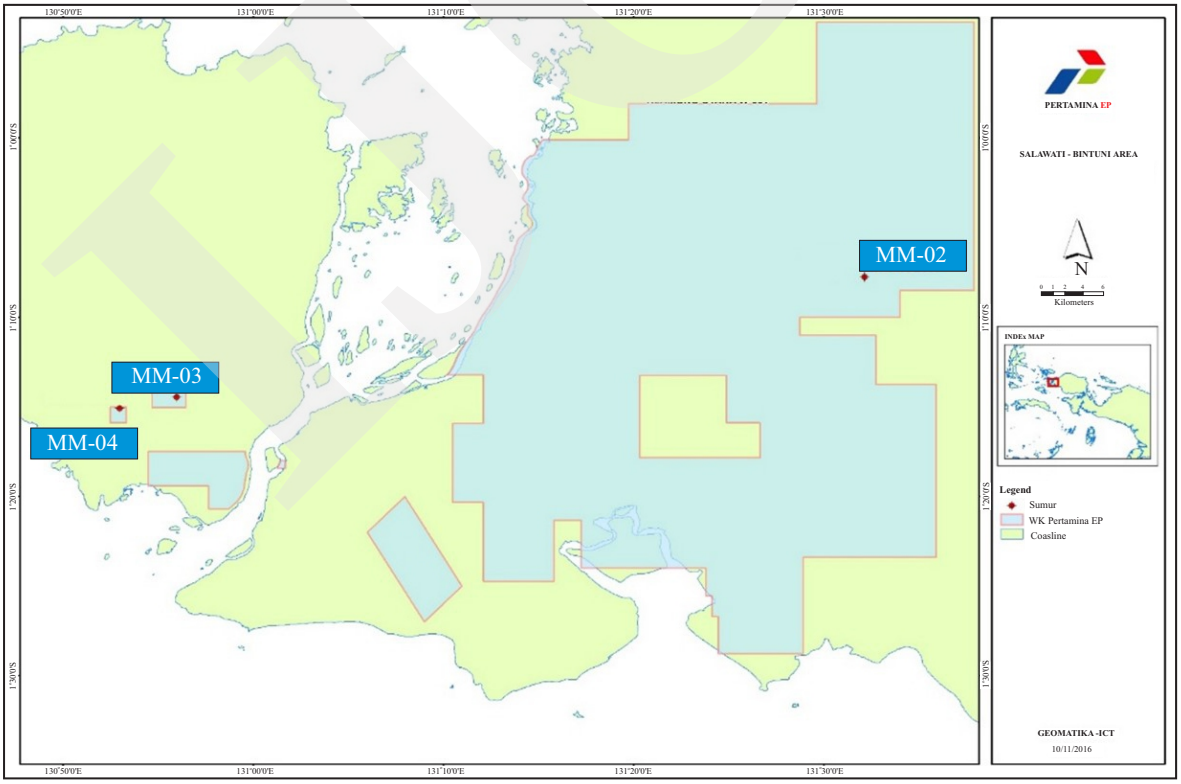


Figure 1. Location map of three wells in Salawati area.

Geological/Stratigraphical Settings

Salawati Basin is geologically bounded by several structures, including the horizontal fault of Sorong Fault which borders the northern part of this basin, between the Australian Continental Plate and Pacific Ocean Plate. To the east and south, the basin is bounded by Ayamaru Exposure and Misool Onin High elevation, respectively (Figure 2) (Hamilton, 1979).

Tectonically, the movement of these three plates amongst Indo-Australian, Eurasian, and Pacific Plates affect the tectonic deformation in eastern Indonesia, especially in the Bird Head area, Papua. The collision between Indo-Australian Continent Plate to the north with Pacific Ocean Plate moving westward has caused the development of a horizontal Sorong Sinistral Fault since Middle Miocene (Hamilton, 1979). Thus, it is thought to be one of the causes of the formation of Salawati Basin. Sorong Fault Zone extends from east to west of the Bird Head, which affects the formation of Salawati Basin, and it is also assumed to be related to the rotation of the Bird Head (Riadini *et al*., 2012).

The stratigraphy of Salawati Basin from the oldest to the youngest rock structures are starting from Kemum Formation, Aifam Formation, and Mesozoic sedimentary rocks (Tipuma Formation and Kembelangan Group), Waripi Formation, Faumai Formation, and Sirga Formation (Satyana, 2008) (Figure 3). Previous researchers Pieters *et al*. (1985) and Atmawinata *et al*. (1989) have mapped the Mawi Complex, located between the Mesozoic Kembelangan Group and the Kemum Formation. Then Saputra, S.E.A. and Fergusson, C.L., (2023) have also carried out new mapping along the Manokwari-Bintuni Road, which allows further division into the Mawi Complex and Tipuma Formation

Kemum Formation (metasediments-metamorphics), which is the basement in Salawati Basin, is a Siluro-Devonian age and the oldest rock in this basin. On top of the basement of Kemum Formation, there is an Aifam Formation which is a Permian carbonate rock, along with Tipuma Formation and

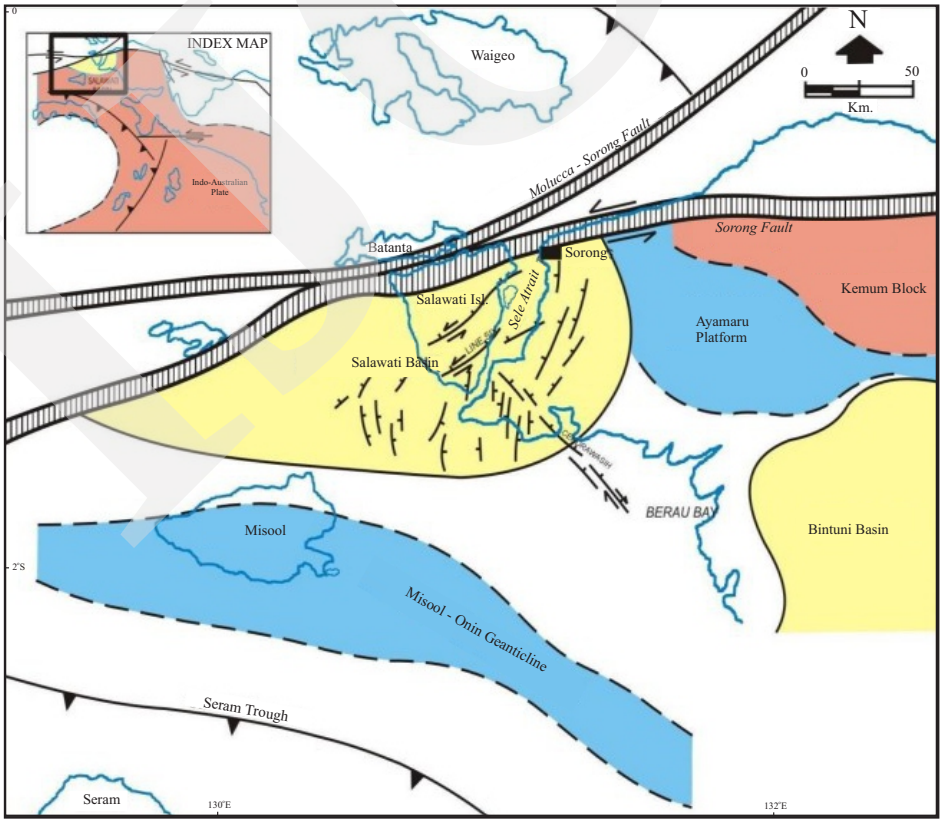


Figure 2. Tectonic map in Bird Head (Hamilton, 1979).

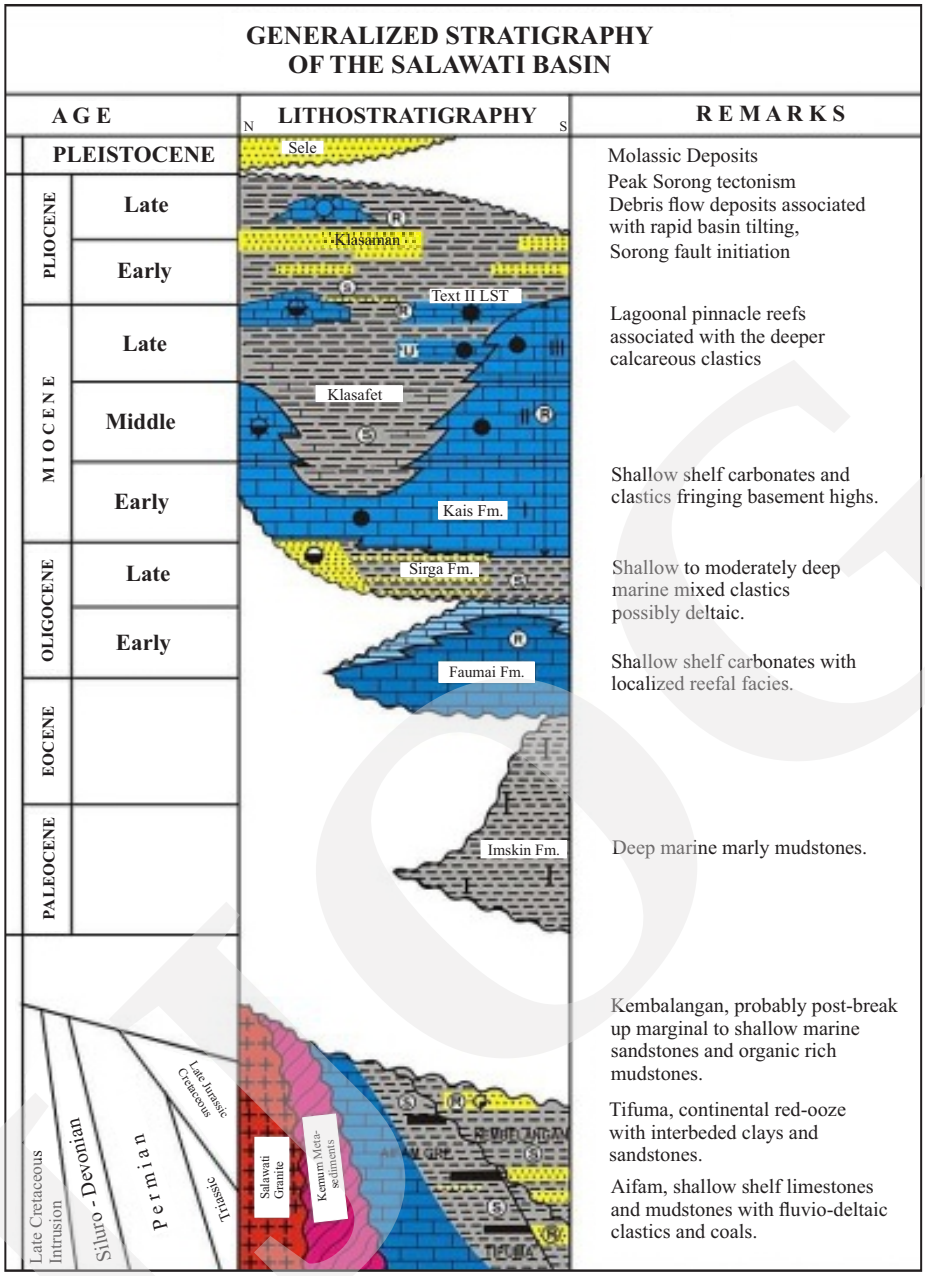


Figure 3. Stratigraphy of the Salawati Basin, West Papua (Satyana, 2008).

Kembelangan Group which are the Mesozoic age.

During the Late Eocene−Early Oligocene period, carbonate deposition began from Waripi, Faumai, and Sirga Formations. Thick carbonates of Kais Formation developed during Miocene age, along with the development of shale from Klasafet Formation at the same time. At the youngest age, the thick layers of shale and sandstones from Klasaman Formation developed during Pliocene period.

The petroleum system formed in the Salawati Basin consists of several parts: source rock, reservoir rock, trap rock, type of trap, and overburden rock (Figure 4). According to Satyana (2010), proven source rocks include the Kais, Klasafet, and Klasaman Formations, with Kais Formation as a proven reservoir rock, and Faumai, Sirga, and Klasaman Formations as unproven reservoir rocks. The cap rocks that are proven in this basin are also the rocks that cause overburden, found in the Kais, Klasafet, Klasaman and Sele Formations. The types of traps that exist in this petroleum system are stratigraphic and structural traps.

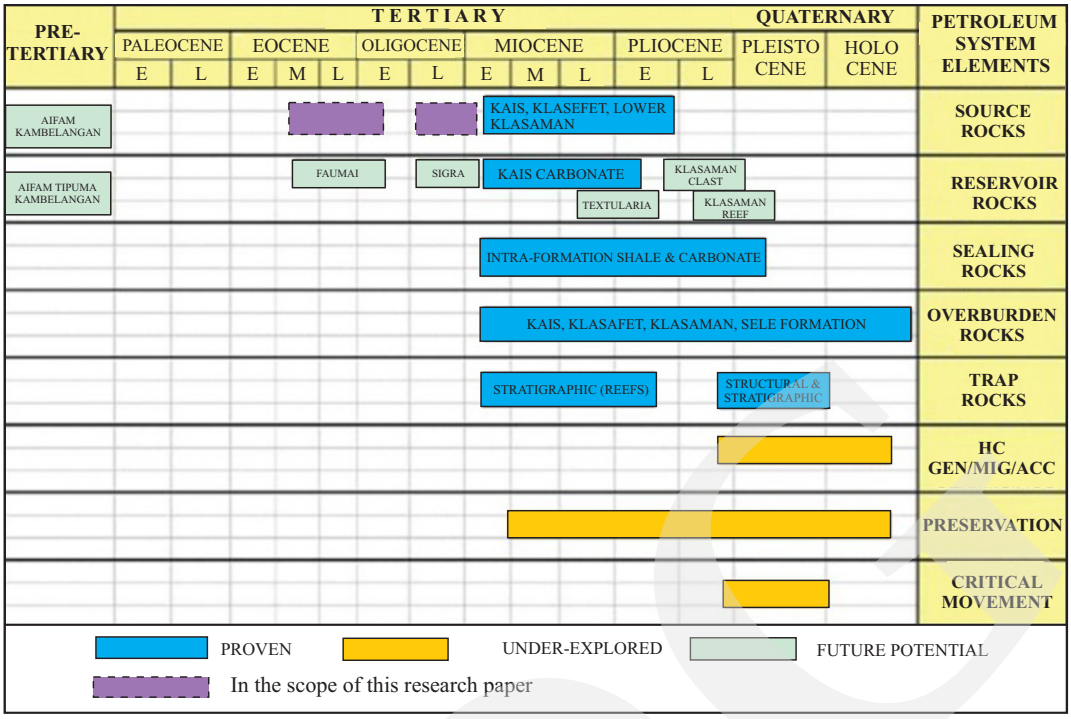


Figure 4. Petroleum system events in Salawati Basin (Satyana, 2010).

Materials and Methods

The research was carried out on three wells in the western part of the Salawati Basin, namely wells MM-02, MM-03, and MM-04 (Figure 1), with the focus on Sirga Formation which is penetrated by these three wells. The method used in this study is organic geochemistry to evaluate the characteristics and the maturity of the source rock. In accordance with the international standard method used by P.T. Geoservices (ISO: 9001: 2015), the type of data used in this study consisted of geochemical data processed in the laboratory, in the form of 13 Total Organic Carbon (TOC), Rock-Eval Pyrolysis (REP), vitrinite reflectance (% Ro), kerogen type, gas chromatography (GC), which continues on the analysis of phenanthrene aromatic biomarkers using gas chromatography/ mass spectrometry (GC/MS) methods. Gas chromatography/mass spectrometry (GC/MS) is a technique used to identify and to measure compounds that are present in low concentrations that can not be adequately separated, identified, and quantified when using gas chromatography (Waples and Curiale, 1999).

Maturation determination in this study has been based on aromatic hydrocarbon parameters, such as trimethylnaphthalene ratio (TNR), methylphenanthrene index (MPI), and dimethylnaphthalene ratio (DNR). These indicators have an advantage of being able to provide information with high maturity; in this case beyond the oil window (Ro: 0.60 - 1.35 %), up to the condensate and dry gas phases (Radke *et al*., 1982; Alexander *et al*., 1985; Kvalheim, 1989).

The selected maturity parameters have a good sensitivity to the determination of thermal maturity including phenanthrene (P), in addition to the MPI (methylphenanthrene index) parameter. The MPI was calculated using the peak areas of P and methylphenanthrene (MP) from mass chromatograms m/z 178 and m/z 192, respectively. The other maturity parameters are based on % Ro and plot diagram of the methylphenanthrene maturity parameters between parameter % Ro equivalent to the MP Index.

According to Radke and Welte (1983), there are two formulas for calculating the maturity value obtained from the analysis of phenanthrene biomarkers, those are:

$$Rc^1 = 0.6\,MPI\text{-}1 + 0.4 \quad \text{.....(1)}$$

$$Rc^2 = 0.99\,[\log_{10} MPI\text{-}2] + 0.94 \quad \text{.....(2)}$$

The thermal maturity formulas by Kvalheim *et al.* (1987) are:

$$R_o^1 = -0.166 + 2.242F_1 \quad \text{.....(3)}$$

$$R_o^2 = -0.112 + 3.739F_2 \quad \text{.....(4)}$$

which are:

$$F_1 = \frac{2\text{-MP} + 3\text{-MP}}{2\text{-MP} + 3\text{-MP} + 1\text{-MP} + 9\text{-MP}}$$

$$F_2 = \frac{2\text{-MP}}{2\text{-MP} + 3\text{-MP} + 1\text{-MP} + 9\text{-MP}}$$

Samples with different maturity can be shown from the methylphenanthrene ratio (MPR). The parameters for the MPI, MPR, and F calculation equations are as follows:

$$MPI\text{-}1 = \frac{1.5*[2\text{-MP} + 3\text{-MP}]}{P + 1\text{-MP} + 9\text{-MP}} \qquad MPR\text{-}1 = \frac{2\text{-MP} + 3\text{-MP}}{1\text{-MP}}$$

$$MPI\text{-}2 = \frac{3*[2\text{-MP}]}{P+1\text{-MP}+9\text{-MP}} \qquad MPR\text{-}2 = \frac{2\text{-MP}}{9\text{-MP}}$$

$$F_1 = \frac{2\text{-MP} + 3\text{-MP}}{2\text{-MP} + 3\text{-MP} + 1\text{-MP} + 9\text{-MP}} \qquad F_2 = \frac{2\text{-MP}}{2\text{-MP} + 3\text{-MP} + 1\text{-MP} + 9\text{-MP}}$$

These various parameters of maturity level were then validated using the K-Means Clustering method. K-Means Clustering is an unsupervised machine-learning method that has the basis for grouping centroids on a set of parameters. This algorithm aims to minimize cluster performance index, square-error, and error criterion (Li and Wu, 2012). The K-means algorithm searches for a predetermined number of clusters within an unlabeled multidimensional dataset (VanderPlas, 2017). The K-means clustering algorithm was used for partitioning a dataset with n observations into K (classes) distinct clusters centred at a centroid (Pandey *et al*., 2020). It allows efficient exploration of multidimensional data by organizing it into meaningful clusters. This aids in uncovering patterns and trends that may not be immediately apparent in the raw data.

Result and Discussion

The GC/MS result analysis obtained from aromatic biomarker ion phenanthrene (P) and methylphenanthrene (MP) index parameters were gained from mass chromatograms m/z 178 and m/z 192 at a well depth that was assumed to be representative, namely well MM-2 (depth 1,416 – 1,418 m; Figure 5), well MM-3 (3,773 m; Figure 6), and MM-4 (3,359 m; Figure 7), were in the form of several parameters of thermal maturity, including MPI, MPR, F1, F2, Ro1, Ro2, Rc1, and Rc2 (Table 1). Then by using Radke and Welte (1983) and Kvalheim *et al*. (1987) formulas, the % Ro value of these parameters could be determined.

The thermal maturity value obtained from Radke and Welte (1983) and Kvalheim *et al*. (1987) formulas is compared to % Ro value

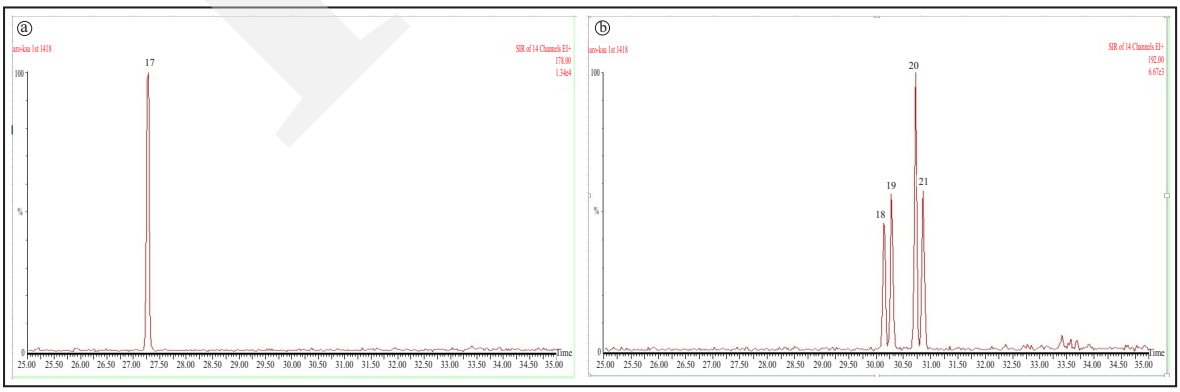


Figure 5. Biomarker fingerprints with ion masses (a) m/z 178 phenanthrene (P) and (b) m/z 192 methylphenanthrene (MP) with a depth of 1416 – 1418 m; extract samples (Sirga Formation) from Well MM-02.

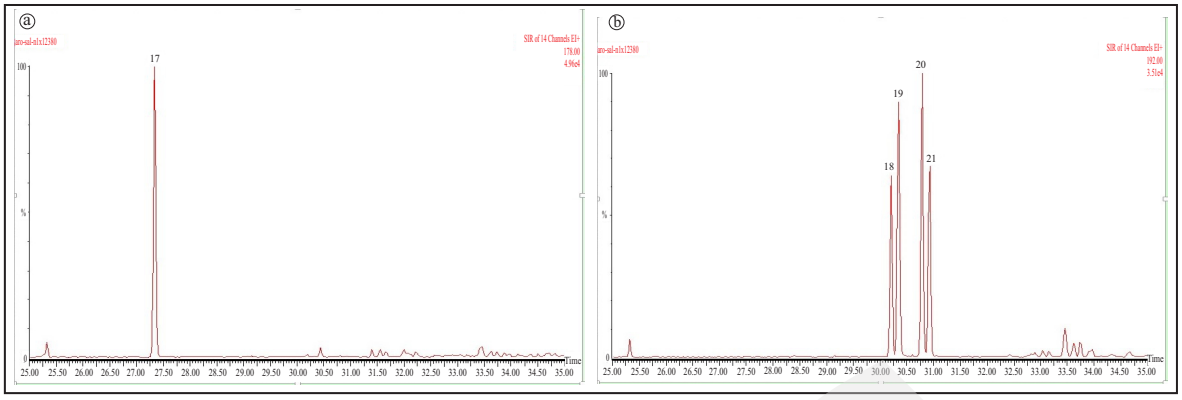


Figure 6. Biomarker fingerprints with ion masses (a) m/z 178 phenanthrene (P) and (b) m/z 192 methylphenanthrene (MP) with a depth of 3,773 m; extract samples (Sirga Formation) from Well MM-03.

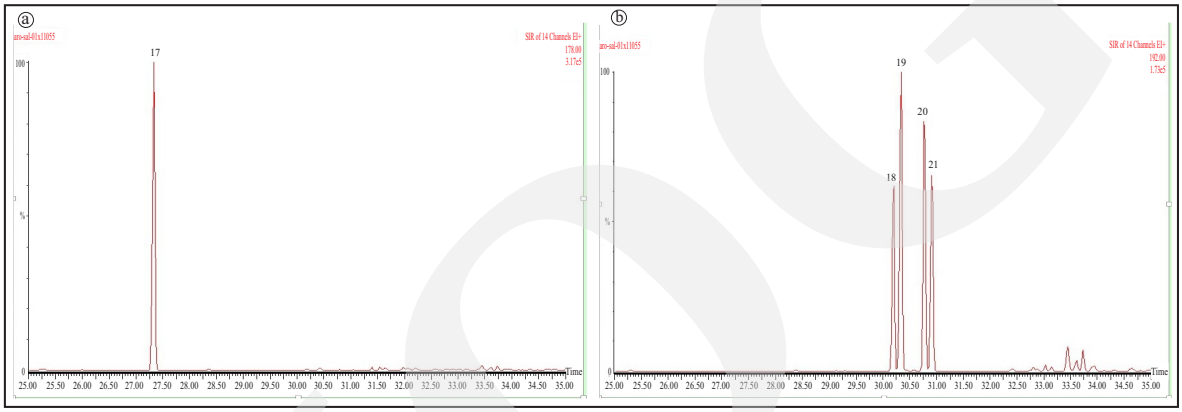


Figure 7. Biomarker fingerprints with ion masses (a) m/z 178 phenanthrene (P) and (b) m/z 192 methylphenanthrene (MP) with a depth of 3,359 m; core sample (Sirga Formation) from Well MM-04.

Table 1. Comparison of Radke and Welte (1983), and Kvalheim *et al.* (1987) Maturity Values on % Ro Laboratory Results

No	Depth (metre)	Type of sample	Ro1	Ro2	Rc1	Rc2	F1	F2	MPR	MPI	Ro_Lab	Formula Radke (1983)	Formula Kvalheim (1987)	Kmeans
0	1386	Cutting	0.71	0.6	0.65	0.6	0.39	0.22	0.56	0.42	0.56	0.65	0.6	2
1	1400	Cutting	0.8	0.71	0.73	0.71	0.43	0.24	0.73	0.54	0.58	0.73	0.71	2
2	1416	Cutting	0.81	0.72	0.71	0.72	0.44	0.26	0.86	0.52	0.6	0.71	0.72	2
3	3711	Cutting	0.88	0.83	0.81	0.84	0.46	0.28	0.88	0.68	0.64	0.81	0.83	1
4	3773	Cutting	0.91	0.84	0.85	0.87	0.48	0.28	0.9	0.75	0.66	0.85	0.84	1
5	3359	Core	0.81	0.7	0.72	0.81	0.44	0.24	0.76	0.54	0.64	0.72	0.7	2
6	3360	Core	0.95	0.89	0.83	0.84	0.5	0.3	1.07	0.71	0.65	0.83	0.89	1
7	3360	Core	0.83	0.8	0.78	0.89	0.44	0.27	0.91	0.63	0.58	0.78	0.8	1
8	3361	Core	0.92	0.87	0.81	0.9	0.48	0.29	1.05	0.69	0.6	0.81	0.87	1
9	3362	Core	0.89	0.8	0.83	0.91	0.47	0.27	0.92	0.71	0.62	0.83	0.8	1
10	3363	Core	0.93	0.86	0.81	0.93	0.49	0.29	1	0.68	0.64	0.81	0.86	1
11	3365	Core	0.91	0.85	0.8	0.95	0.48	0.28	0.95	0.66	0.62	0.8	0.85	1
12	3365	Core	0.92	0.72	0.82	0.96	0.5	0.5	0.81	0.71	0.64	0.82	0.72	1
13	3366	Core	1	0.97	0.84	1.01	0.52	0.52	1.2	0.73	0.56	0.84	0.97	3

from the laboratory observation. The value of % Ro (Table 1) is the result of microscope reading, therefore % Ro is the most accurate parameter (Muhartanto *et al*., 2019).

Muhartanto *et al*. (2019) stated that the results of calculations using Radke and Welte (1983) formula were closer to the % Ro results of the laboratory results, with a difference of % Ro

between 0.09 to 0.15 % (well MM-02), 0.17 to 0.19 % (well MM-03), and 0.08 to 0.28 % (well MM-04). The calculation using Kvalheim *et al*. (1987) formula has a difference between the calculated value with the % Ro value of the laboratory results ranging from 0.04 to 0.13 % (well MM-02), 0.18 to 0.19% (well MM-03), and 0.06 to 0.41 % (well MM-04).

The plot graph between the methylphenanthrene index (MPI) against the % Ro equivalent shows that the thermal maturity will increase with the increasing depth (Figures 8 - 10). Well MM-02

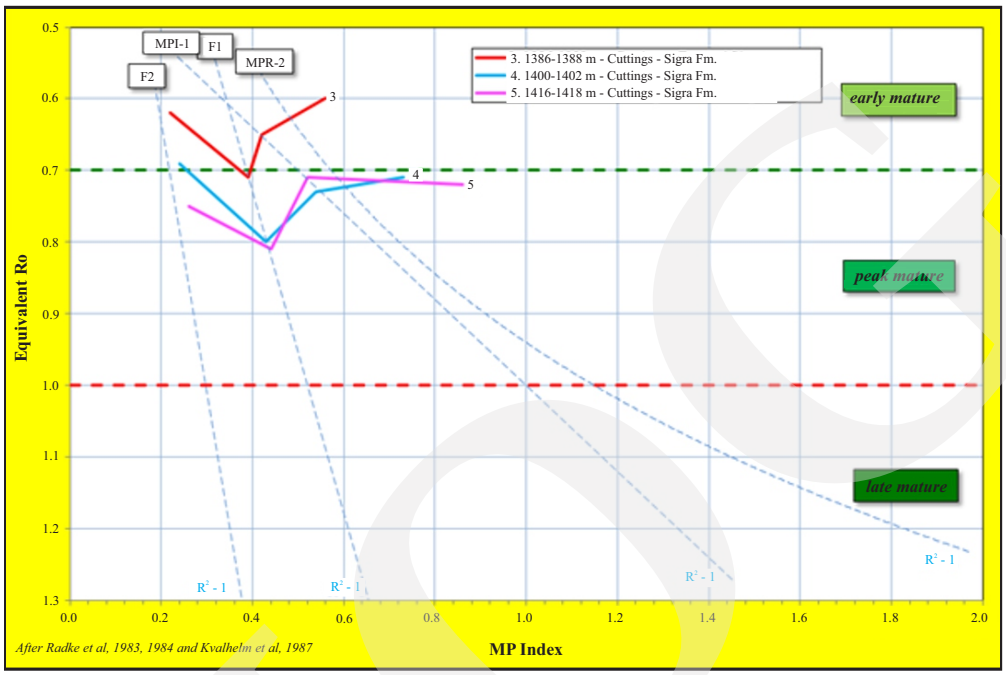


Figure 8. Plot of methylphenanthrene maturity parameters in well MM-02.

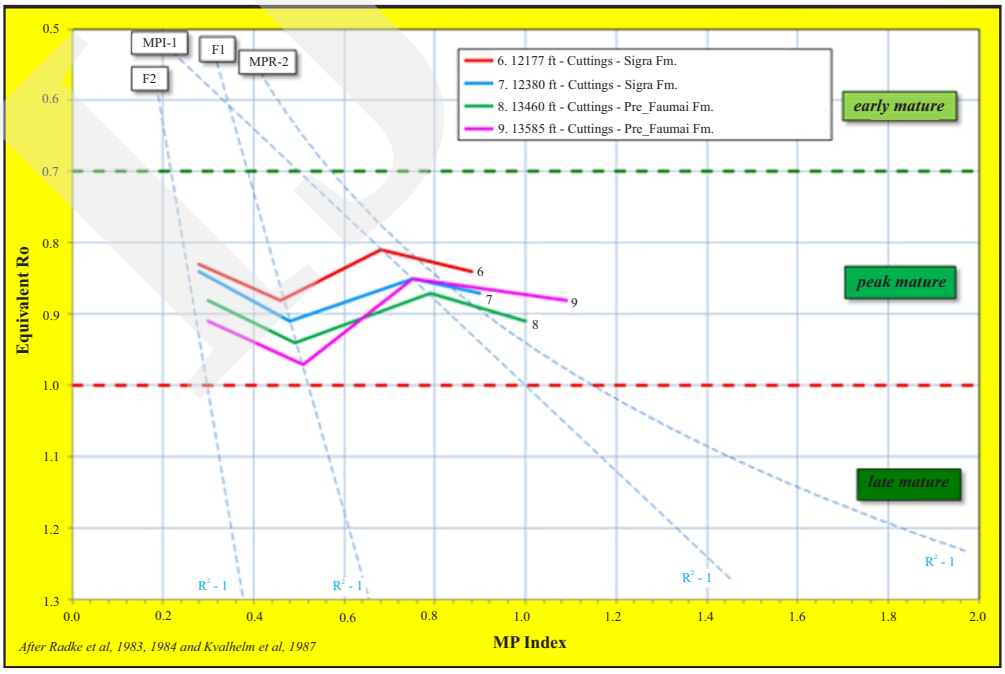


Figure 9. Plot of methylphenanthrene maturity parameters in well MM-03.

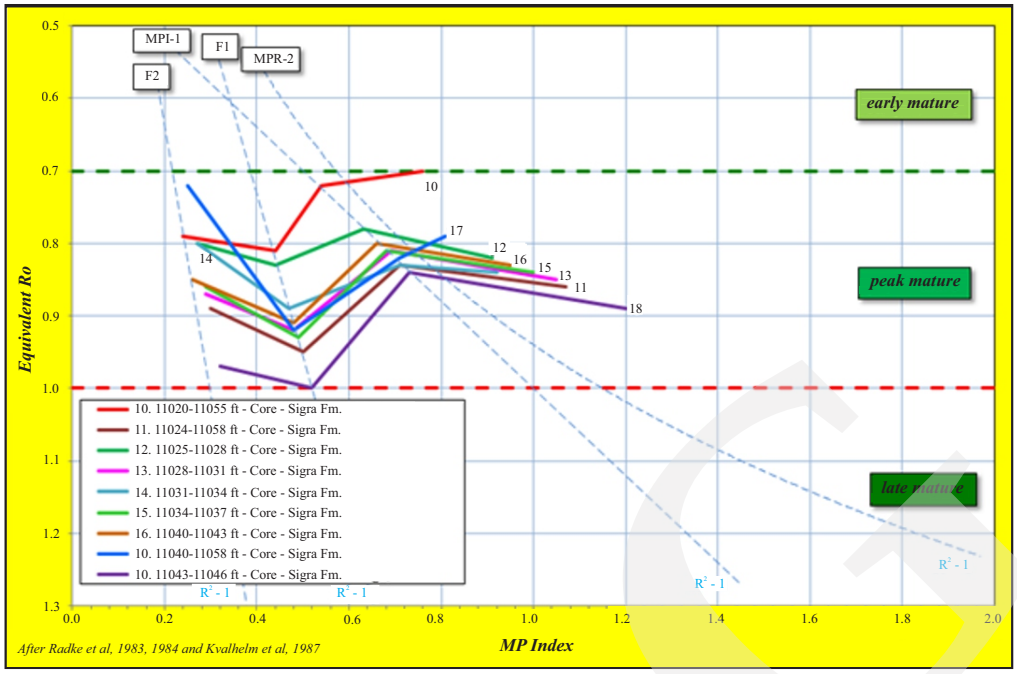


Figure 10. Plot of methylphenanthrene maturity parameters in well MM-04.

has reached early to peak maturity level (Figure 8), well MM-03 has reached peak maturity level (Figure 9), and well MM-04 has reached early – peak maturity level (Figure 10).

Statistical tests were carried out using these parameters based on the maturity of several parameters overall identification. The parameters used include Rc1, Rc2, Ro1, Ro2, F1, F2, MPR, MPI, and depth (Tabel 1). K-means cluster was used as a method for validity test.

The K-means algorithm works by randomly selecting k points from the geochemical dataset as initial cluster centroids. Then, each data point in the dataset is assigned to the cluster whose centroid is closest to it. After all data points have been assigned to a cluster, the centroid of each cluster is recalculated as the mean of all the data points assigned to that cluster. This process of reassigning points to clusters and recalculating the centroids is repeated until the cluster assignments no longer change or a maximum number of iterations is reached.

Regarding this validity test, a cluster model is carried out as described in Table 1, and compared also with Figures 11 and 12. It finally divides the number of K (classes) in the clustering into three groups/classes, later representing the level of maturity columns, namely:

1. Group (zone) sample with peak maturity (class-1 with a black dot).
2. Group (zone) of a sample with early maturity (class-2 with a red dot).
3. *Outlier* (class-3 with a yellow dot).

Based on the data classification which resulted in three groups, it will assume that this method supports the maturity level of data samples in the researched area (Figures 11 and 12).

Based on the appearance of the crossplot (Figure 11), both Radke and Kvalheim Formulas show that the maturity in the studied area is divided into three main zones, namely peak maturity zone, early maturity zone, and outliers. Grouping (clustering) using Radke and Welte Formula (1983) (Figure 11b) is clearer than Kvalheim *et al*. (1987) (Figure 11a) Formula. This supports what has been stated in previous studies (Muhartanto *et al.,* 2019), that the calculation of maturity using Radke and Welte (1983) is more suitable to use in Salawati Basin, West Papua, than Kvalheim *et al*. (1987).

Comparing the results of a crossplot to thermal maturity, both Radke and Welte (1983) and

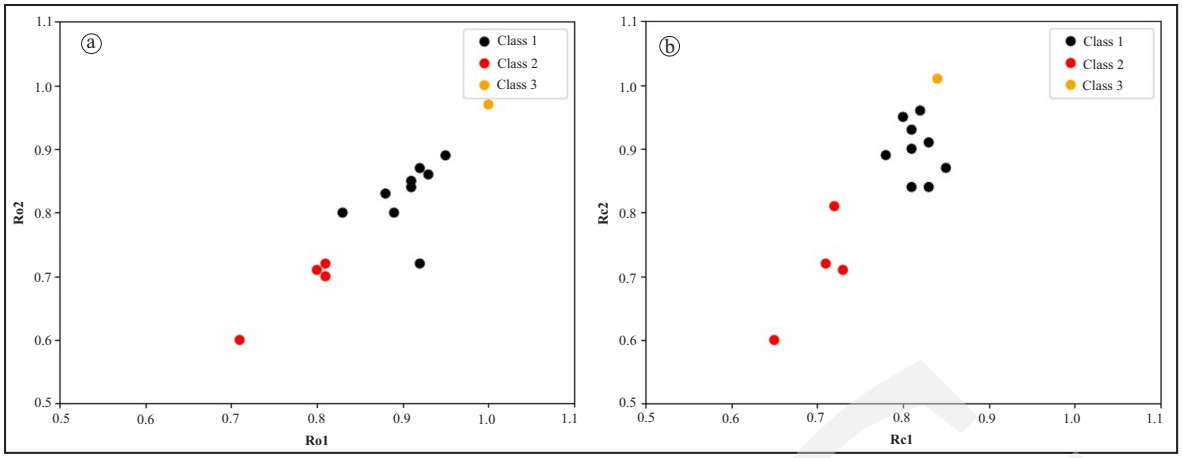


Figure 11. Crossplot between maturity levels of (a) Ro^2 vs Ro^1 (Kvalheim *et al.* 1987) and (b) Rc^2 vs Rc^1 (Radke and Welte, 1983).

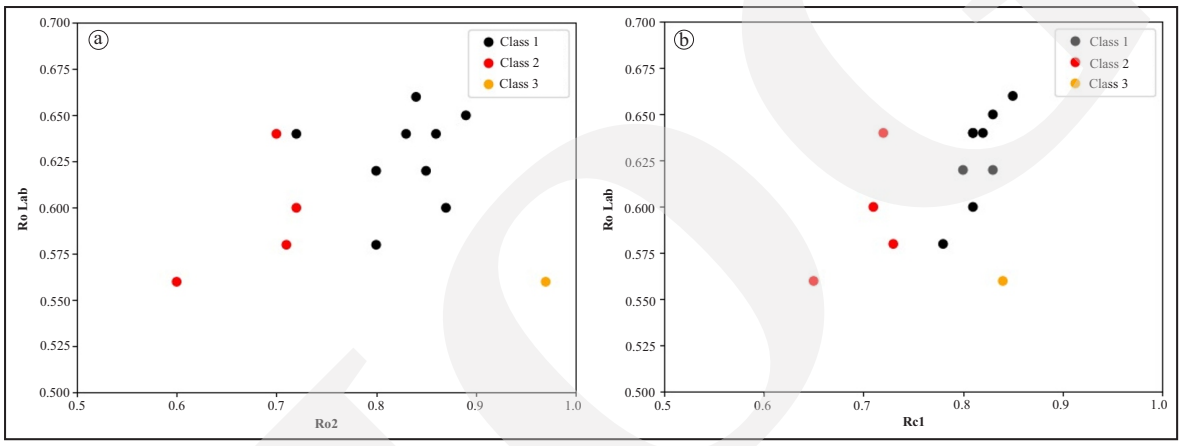


Figure 12. Crossplot between maturity levels of (a) Ro^2 (Kvalheim *et al.* 1987) and (b) Rc^1 (Radke and Welte, 1983) against Ro Lab.

Kvalheim *et al.* (1987) appear to be correlative and close to the Ro Lab maturity value (Figure 12). This assumption raises a new perspective that differs from a previous research (Muhartanto *et al.,* 2019). MPI, Ro lab, Ro2, and Rc1 plots for each depth show a correlation between thermal maturity increase and depth (Muhartanto *et al.*, 2019). This is supported and shown in the depiction of the crossplot between MPI and Ro Lab below (Figure 13), which proves that an increase

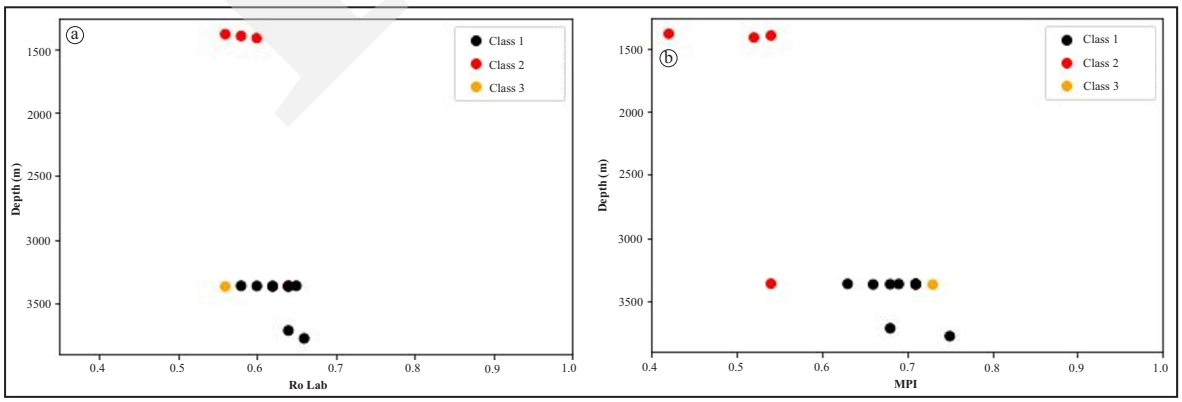


Figure 13. Crossplot between maturity levels of (a) MPI and (b) Ro Lab against depth.

in thermal maturity will always be correlated with an increase in the depth.

The peak maturity values are relatively in the same zone (black zone) with the maturity at adjacent depths (Figure 13). Meanwhile, the early maturity value is shown by the red zone at a relatively shallower depth (Figure 13).

Conclusions

Thermal maturity level based on biomarker methylphenanthrene (MP) shows a maturity that has reached early to peak level. This indicates that there has been hydrocarbon formation (oil generation) in Salawati Basin, West Papua, Indonesia.

The results of the laboratory analysis regarding the maturity parameters of aromatic hydrocarbons are clearly shown in the graph plot of methylphenanthrene index (MPI) against % Ro equivalent, indicating that as the depth increases, the thermal maturity will also increase. In the MM-02 well, it has reached early to peak the maturity level, well MM-03 has reached peak the maturity level, and well MM-04 has reached the early – peak maturity level.

Based on the clustering zone grouping, there are three thermal maturity zones, namely peak mature, early mature, and outliers. K-means clustering helps in discerning clear boundaries between different maturity levels based on the parameters considered. This allows a more granular understanding of the data.

The K-means clustering method supports and proves that increasing thermal maturity will always correlate with increasing depth.

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