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To cite this article: A. E. Chemodanov, R. R. Akhmadullin, V. A. Sudakov, S. A. Usmanov & R. K. Khayrtdinov (2018) Geochemical modeling with the use of vertical and horizontal relative concentrations of oil compounds for the heavy oil fields, *Petroleum Science and Technology*, 36:14, 1100-1106, DOI: [10.1080/10916466.2018.1463251](https://doi.org/10.1080/10916466.2018.1463251)

To link to this article: <https://doi.org/10.1080/10916466.2018.1463251>



Published online: 07 May 2018.



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# Geochemical modeling with the use of vertical and horizontal relative concentrations of oil compounds for the heavy oil fields

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## ABSTRACT

The purpose of this study is to detect lateral and vertical gradients of relative concentrations of compounds presented in oil, which allows assessing potential drainage zones in the reservoir during the reservoir production by steam injection. In this research new method for monitoring of steam chamber development in 2D model was created and tested. Methodology: Total hydrocarbon fraction was isolated from core extracts and analyzed by GCMS method (TIC) for detection of various compounds and assessment of lateral and vertical gradients of their concentration in lateral. It was found that the ratio of 4- and 1-methyldibenzothiophenes (MDBT) changes in lateral and in vertical directions. These changes are caused by biodegradation of organic matter. Laboratory research shows that 1-MDBT/4-MDBT ratio in native reservoir rocks is stable under high temperatures and pressure and can be easily measured by GC-MS. This measurement will allow assessment of location and direction of steam chamber propagation. In recent work the authors have developed geochemical model which can be used for assessment of oil flow directions during the development of heavy oil fields by SAGD method.

## KEYWORDS

biodegradation of oil; heteroatomic compounds; isomers; oil-water transition zone; SAGD modeling

## 1. Introduction

The development prospects of the oil industry recently have been linked to the development of deposits of heavy oil and natural bitumen (Sitnov 2016; Vakhin 2016). In the mid-1980s, Canada developed a SAGD-Steam-Assisted Gravity Drainage technology (Butler 1991).

There is a large number of works have been published about the modeling of developing superviscous oil deposits using the SAGD method, but many of the parameters characterizing the nature of the reservoir and the basic properties of the oil have been simplified. This may cause significant differences in the model and the real object it describes, which will lead to not adequate prediction of the oil production process.

One promising solution to this problem is the geochemical modeling of the fields, based on the study of the zonation of composition and the properties of the oil in the deposit. As we know, any oil contains a unique set of compounds; the ratio between them can both maintain constant values throughout the reservoir as well as show lateral and horizontal gradients. The zoning of the composition and properties of oil in shallow deposits is mainly associated with the bio-degradation of organic compounds and is significantly different from the changes caused by physical processes such as washing out and fractionation. For example, Bennett and Adams (2013) shows that hopanes, methyladamantanes do not have horizontal gradients by the content, while the concentration of mono-, di- and tri-aromatic hydrocarbons



(including heteroatomic) decreases with depth. Chemodanov et al. (2017) demonstrated that concentration 6H-Farnesol in oil may be increase with depth. Specifying dependency of the distribution of any compounds over the whole field will certainly clarify the location and direction of the steam chamber by using GCMS analysis of the extracted oil.

Thus, the establishment of a method for monitoring the development of deposits by natural oil markers is a matter of urgency, which will make it possible to clarify existing patterns of deposits and improve their predictive capacity.

The purpose of this work is to identify the gradients of ratios of compound molecules and show their possible use for the development of superviscous oil deposits in the case of the Nizhne-Karmal'skoe anticline of the Cheremshanskoe oil field (Tatarstan, Russia), where the SAGD technology is currently being used.

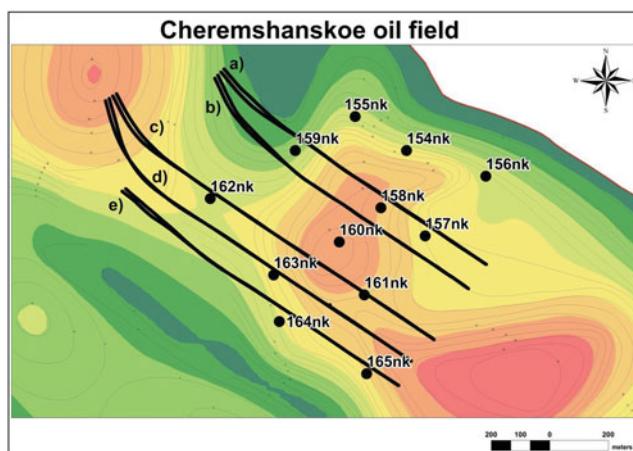
## 2. Materials and methods

The research objects are core samples, selected from the 12 assessment wells of the Nizhne-Karmal'skoe anticline of the Cheremshanskoe oil field **Figure 1**.

The results of the macro description of core show that the oil reservoir being studied has one layer in the entire field, but its depth and thickness vary greatly. The core samples were selected on the whole thickness of the productive reservoir, if possible at the same intervals. As a result, the number of core samples selected from the appraisal wells ranged from 3 to 6 per well, and the thickness of the sampling interval were 4–8 meters, depending on the thickness of the oil reservoir **Table 1**. The upper and lower samples were selected as close as possible to the top and the base surface of the reservoir.

The extraction of bitumen using chloroform was carried out using the Soxhlet extractor. The hydrocarbon fraction, containing saturated and aromatic hydrocarbons, provided using a method of liquid-absorbed chromatography on the siliceous gel (0.25–0.5 mm fraction). Petroleum-ether was used as a movable phase.

The hydrocarbon fraction of bitumen and oil was examined on the gas chromatography/mass-spectrometer system, which included the gas chromatograph "Chromatech-Crystal 5000" with a mass-selective detector ISQ (USA). The Xcalibur software have been used for processing the results. The chromatograph is fitted with a capillary column, 30 m long, with a diameter of 0.25 mm. The speed of the flow of carrier gas (helium) — 1 ml/min. The injection temperature is 310°C. The temperature program of the thermostat is a rise from 100 to 150°C at a speed of 3°C/min, from 150 to 300°C at a speed of 12°C/min followed by its isotherm to the end of the analysis. Electron energy — 70 eV, temperature of



**Figure 1.** Location of the appraisal and horizontal wells of the Nizhne-Karmal'skoe anticline of the Cheremshanskoe oil field (Tatarstan, Russia).

**Table 1.** The number of core samples selected from the assessment wells.

No	Well	Depth of the oil reservoir, m			Number of samples
		Top	Base surface	Thickness	
1	154	131.5	154.1	22.6	4
2	155	145.4	156.2	10.8	3
3	156	129.6	158.2	28.6	4
4	157	124.4	160.0	35.6	6
5	158	130.2	160.3	30.1	5
6	159	151.8	168.3	16.5	3
7	160	137.1	170.0	32.9	6
8	161	129.8	168.8	39.0	5
9	162	171.0	179.0	8.0	3
10	163	150.0	174.3	24.3	4
11	164	149.8	182.3	32.5	5
12	165	132.6	162.6	30.0	4
					Total 52

ion source — 250°C. The compounds have been identified through the electronic library of the NIST spectra and according to the data of the literary sources.

### 3. Results and discussion

The chromatography-mass-spectrometric analysis of hydrocarbon fractions shows the absence of normal alkanes and the dominance of isoprenoid hydrocarbons in all samples **Table 2**.

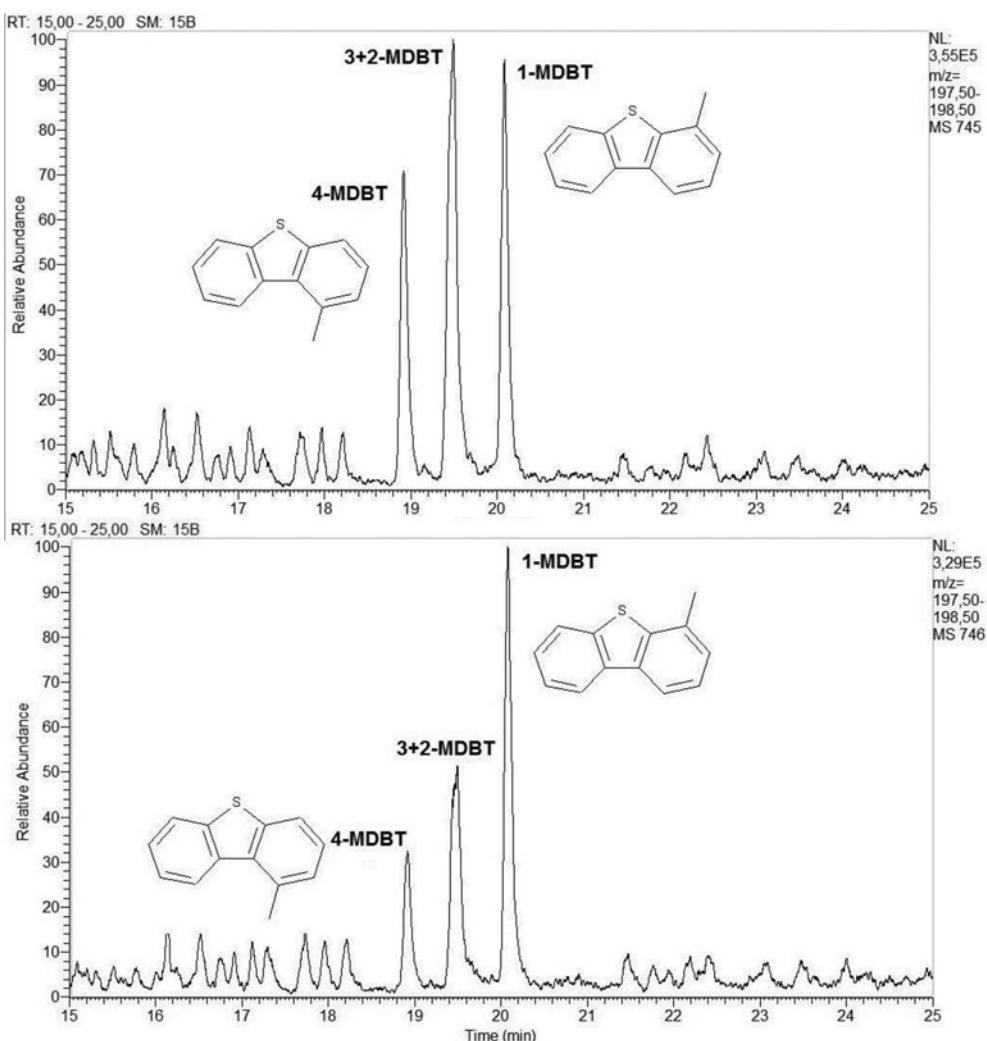
The absence of n-alkanes in the core sample indicates about degradation of organic matter. There exist two classical scales of oil bio-degradation, namely Peters-Moldowan (Peters and Moldowan 1993) and Wenger (Wenger, Davis, and Isaksen 2002) scales, based on which ones can assess approximate depth of biological destruction of organic matter. Both scales provide for the assessment of the availability of n-alkanes, isoprenoids, steranes and hopanes. The Wenger scale, unlike the Peters-Moldowan scale, also includes the identification of di- and tri-aromatic compounds.

**Table 2** shows that, apart from the lack of n-alkanes, which we can observe on the total ion current, there are no C0-C2-Naphthalenes in the specimens studied, although C3- and C4-naphthalenes are still identifiable. It is also worth noting the presence of monoaromatic hydrocarbons, hopanes and steranes. On the basis of the results of the gas chromatography/mass analysis, we conclude that organic matter in the specimens is moderately biodegraded on the Peters-Moldowan scale (4–5 units) or heavily biodegraded on the Wenger scale (3 units).

It is necessary to determine which components surviving in the biodegradable environment are characterized by gradients of relative concentrations throughout the deposit. Relative concentrations

**Table 2.** Results of the GCMS (gas chromatography-mass spectrometry) analysis of hydrocarbon fractions of bitumen.

Compound	m/z	Presence (+/–)	Note
N-alkanes	85	–	Not found even in trace amounts
Isoprenoid alkanes	85	+	The contents vary between 60 and 90% rel. (78% on average for all samples)
Monoaromatic hydrocarbons	91, 133	+	The content varies between 2 and 20% rel. (10% on average for all samples)
Naphthalene	128	–	–
Monomethylnaphthalene	142	–	–
Dimethylnaphthalene	156	–	–
Trimethylnaphthalene	170	+	–
Tetramethylnaphthalene	184	+	–
Steranes	217	+	The main sterane and hopane geochemical coefficients are the same for all specimens
Hopanes	191	+	



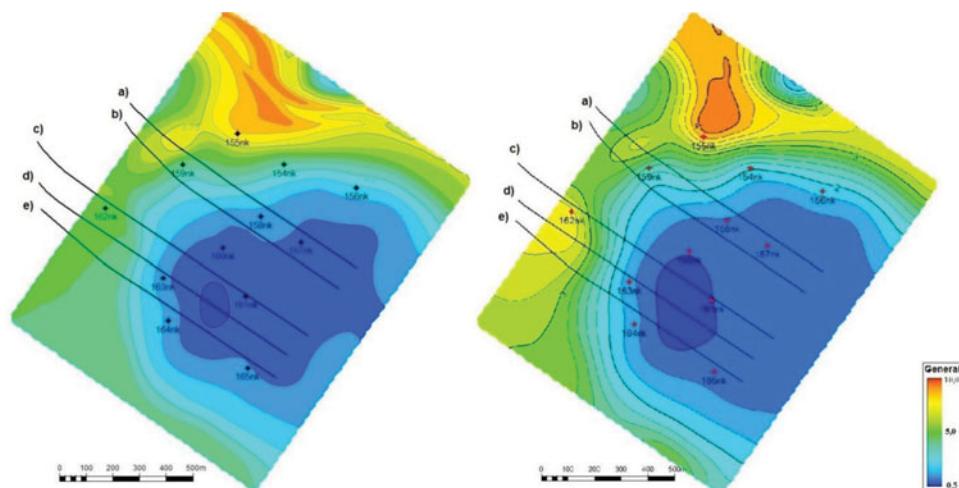
**Figure 2.** Mass-chromatograms ( $m/z = 198$ ) of various samples of the well No. 163.

of isoalkanes, aromatic hydrocarbons, hopanes and steranes do not have any patterns in the distribution of the prospect.

As you know, heteroatomic compounds are quite resistant to the processes of degradation (Peters, Walters, and Moldowan 2005). Two of these compounds, which are present in all samples studied, are 1- and 4-methyldibenzothiophenes. Bennett, Adams, and Larter (2009) have shown that 4-methyldibenzothiophene (4-MDBT) was less resistant to degradation than 1-methyldibenzothiophene (1-MDBT), so that the ratio 1-MDBT/4-MDBT is an indirect indicator of the degree of degradation of organic matter. Figure 2 shows mass-chromatograms (by  $m/z = 198$ ) of two samples of the well No. 163 core, indicating the peaks 1-MDBT and 4-MDBT.

For all core samples, a ratio of 1-MDBT/4-MDBT, which varies in the range of 0.4–11.0 (Table 3), has been defined. Average values of 1-MDBT/4-MDBT on wells lie between 0.6 and 9.4.

According to the lateral distribution of the average ratios 1-MDBT/4-MDBT, the geochemical 2D models of the area of the deposit Figure 3 were constructed using Schlumberger Petrel 2013 software. Zones with low values of 1-MDBT/4-MDBT are colored blue and dark blue, and the zones with high ratio are yellow and red. It should be noted that we have a reasonably accurate model using data from



**Figure 3.** Lateral distribution of the average value of 1-MDBT/4-MDBT by area based on data for 6 wells (left) and 12 wells (right). The black lines indicated by the letters (a) to (e) are the horizontal extracting wells.

six wells. Adding six more wells does not radically change the model that was built, but merely makes it more accurate.

According to [Table 3](#), the ratios 1-MDBT/4-MDBT can be quite different even for samples taken from the same well, but from different depths. The vertical distribution of the ratios 1-MDBT/4-MDBT for some of the appraisal wells situated close to the production well is presented in [Figure 4](#). These wells have relatively low values of 1-MDBT/4-MDBT at the top of the productive layer. In the lower part of the oil reservoir there is a sharp increase in the ratio of isomers of methyldibenzothiophenes: at a depth of 150 meters for wells 157, 158 and 160 and at a depth of 160 meters for wells of 160 and 163. It is important to note that this pattern is not characteristic for the well 161, as the entire thickness of its productive layer is low in the values of 1-MDBT/4-MDBT.

The gradients obtained may be related to the presence of oil-water transition zone at a depth of 150–160 meters, where the most intensive biodegradation of organic matter occurs. As the depth of oil decreases, its biological decomposition is also beginning to be suspended. It is also worth noting that the indicator 1-MDBT/4-MDBT correlates with the thickness of the oil reservoir, which is exponential [Figure 5](#), due to the reduction in biological effects while reducing the thickness of the productive layer.

**Table 3.** Values of 1-MDBT/4-MDBT ratio for kern samples from different wells.

Well	Depth of the productive layer, m	1-MDBT/4-MDBT ratio		
		Increase of the sampling depth		Average value of the well
		0.9–0.9–1.9–2.1	8.0–9.2–11.0	
154	131.5–154.1	0.9–0.9–1.9–2.1	8.0–9.2–11.0	1.5
155	145.4–156.2	1.3–1.3–2.5–0.4	1.3–1.3–2.5–0.4	9.4
156	129.6–158.2	0.5–0.7–0.6–0.7–0.7–1.6	0.6–0.7–0.9–0.7–1.8	1.4
157	124.4–160.0	0.6–0.7–0.6–0.6–0.9–2.2	3.3–2.8–2.7	0.8
158	130.2–160.3	0.6–0.7–0.9–0.7–1.8	0.6–0.7–0.9–0.7–1.8	0.9
159	151.8–168.3	0.6–0.7–0.6–0.6–0.9–2.2	0.6–0.5–0.8–0.9–0.4	2.9
160	137.1–170.0	0.6–0.7–0.6–0.6–0.9–2.2	0.6–0.5–0.8–0.9–0.4	0.9
161	129.8–168.8	0.6–0.7–0.6–0.6–0.9–2.2	0.6–0.5–0.8–0.9–0.4	0.6
162	171.0–179.0	0.6–0.7–0.6–0.6–0.9–2.2	1.2–5.3–8.7	5.1
163	150.0–174.3	0.6–0.7–0.6–0.6–0.9–2.2	1.0–1.2–1.1–2.8	1.5
164	149.8–182.3	0.6–0.7–0.6–0.6–0.9–2.2	0.9–1.1–1.1–2.6–2.2	1.6
165	132.6–162.6	0.6–0.7–0.6–0.6–0.9–2.2	0.7–0.9–3.5–3.7	2.2

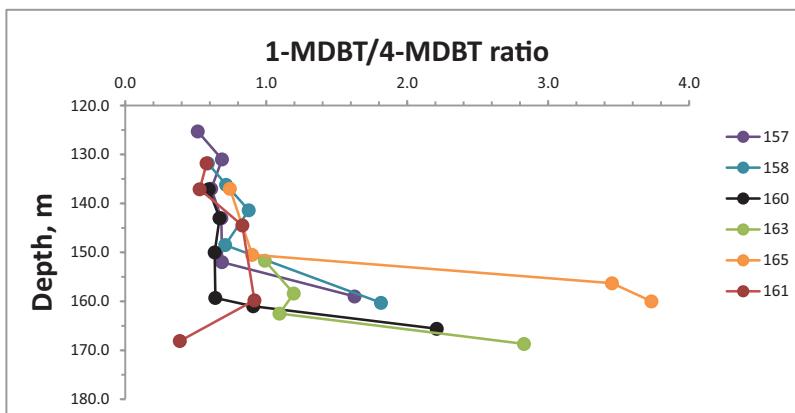


Figure 4. Vertical distribution of 1-MDBT/4-MDBT ratios for some appraisal wells.

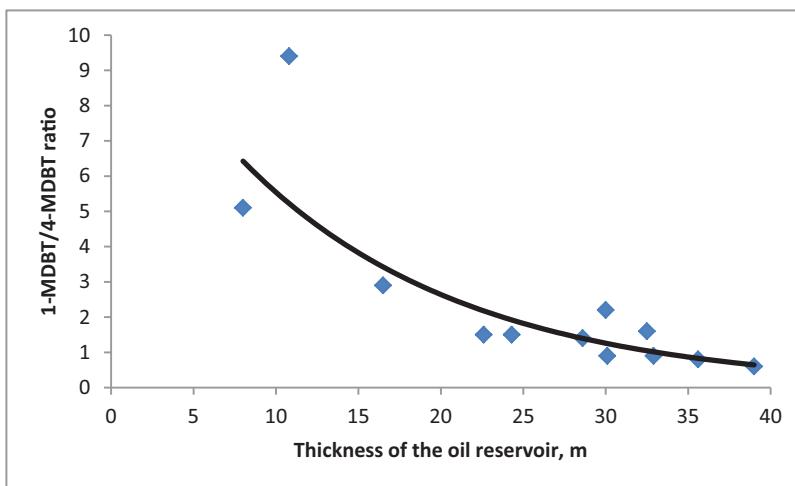


Figure 5. Dependence of average ratio 1-MDBT/4-MDBT of the wells from the thickness of the oil reservoir.

In order to suggest possible ways of inflow of oil to the horizontal wells, samples of the oil from the horizontal wells shown in Figure 1 marked from (a) to (e) were analyzed. The molecular composition of oil hydrocarbon fractions, according to HMS Analysis, showed the same components as found in the core samples Table 2. However, the 1-MDBT/4-MDBT ratios for samples of extracted oil from the horizontal wells showed the different results. The ratio 1-MDBT/4-MDBT for specimens (a), (b), (c) and (e) are roughly the same, 0.5–0.7, which corresponds to the blue zone on the lateral distribution. In addition, for these horizontal wells, we can exclude the shift of the steam camera horizontally down. For sample (d) The 1-MDBT/4-MDBT ratio is 1.6, which indicates that there are inflows of superviscous oil to the production well from the lower part of the productive layer (from a depth of 150–160 meters).

#### 4. Conclusion

In our current study we established the level of biodegradation of organic matter in the Nizhne-Karmal'skoe anticline of the Chermshanskoe oil field. We found the presence of horizontal and lateral gradients of the ratio of methyldibenzothiophenes in the organic matter of the oil reservoir and showed the stability of this ratio in conditions of SAGD process. The presence of these gradients is determined by the depth of the occurrence, the thickness of the oil reservoir, taking into account the location of the

appraisal wells. Within the developed model, it has been shown that the molecular composition of produced superviscous oil suggests possible ways of influx in the development of the deposits by the SAGD method.

## Acknowledgments

The reported study was performed according to the Russian Government Program of Competitive Growth of Kazan Federal University. The work was supported by the Ministry of Education and Science of the Russian Federation (project No. 02.G25.31.0170).

## Funding

This work was supported by Ministry of Education and Science of the Russian Federation (project No. 02.G25.31.0170); Russian Government Program of Competitive Growth of Kazan Federal University.

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