Thermal Effect on the Distribution of Regular Sterane and Geological Significance

Yunfei Yang¹,², Min Zhang¹,²*, Julin Chen¹,², Xiaohui Chen¹,²

¹Key Laboratory of Exploration Technology for Oil and Gas Research (Yangtze University), Ministry of Education, Wuhan, China
²College of Resources and Environment, Yangtze University, Wuhan, China
Email: *zmjpu@163.com

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Abstract

In order to study thermal effect on distribution characteristics of regular sterane in humic coals, a suit of 25 coals derived from Kuqa Depression in Tarim Basin and Ordos Basin are studied to investigate the distribution of regular sterane in different maturity, which mainly discusses the thermal effect. The results show that the C₂₇ααα/C₂₉ααα regular sterane ratio has a linear relationship with Ro (tₘₐₓ) and aromatic hydrocarbon maturity parameters in the coals from mature to high-mature stage. It suggests that the distribution of the C₂₇, C₂₉ regular steranes will fail to reflect original source input in high evolutionary stage. On the basis of thermal simulation experiment results, it further proves that the distribution patterns result from the demethylation effect of C₂₉ regular sterane in the mature to high mature evolution stage and the C₂₇ααα/C₂₉ααα regular sterane increases with increasing maturity. The breakage of C-C key in branched chain from C₂₇, C₂₉ regular steranes to make C₂₇ααα/C₂₉ααα regular sterane ratio invariance at high and over mature stage. Therefore, the ratio can be used to distinguish the maturity in high and over mature stage.

Keywords

Sterane, Maturity, Pyrolysis Experiment, Geochemistry Characteristic, Oil-Rock Correlation

1. Introduction

Sterane refers to the compounds which derive from the animals, plants and other organisms for complex sterol mixture of coal, hydrocarbon source rocks and crude oil species [1]. Because of its special structure containing rich geochemical information, it is often used to study oil source correlation, sedimentary environment, thermal evolution degree, the biodegradation and geological evolution history [2] [3] [4] [5] [6]. So far, these geochemical properties of sterane com-
pounds had been researched by many domestic and foreign scholars. The research has shown that the carbon number distribution of regular sterane is mainly affected by organic matter input, indicating that regular sterane compound could act as powerful source parameters. C27 regular sterane indicates the source of aquatic algae, while C29 regular sterane suggests the source of higher plants. So the relative percentage content of C27, C28 and C29 regular sterane can be frequently used to judge source input and oil source correlation [1] [7] [8]. If the compound of C27 and C29 regular sterane appears on a double peak in the chromatograms, this can be speculated that the organic matter is not only derived from continental deposits but also from marine deposits [9].

In 1975, Alomon studied the influence of clay minerals for oil and gas formation mechanism using pyrolysis experiment [10]. Meanwhile, the relationship of sterane and thermal evolution was studied in the Paris Basin shale, and the maturity parameters of C2920S/(20S + 20R) and C29-ββ/(αα + ββ) regular sterane were first put forward by Mackenzie in 1980 [11]. Because the R configuration on sterane C-20 was considered that it exists only in the precursor of living creatures’ body. With the buried depth and thermal evolution degree increasing, the R configuration gradually converts a mixture of R and S configuration until to balance. After that, the phenomenon of the C29 regular sterane maturity parameter reversing was found in high maturity of hydrocarbon source rocks [12] [13]. In addition, immature hydrocarbon source rocks have done the pyrolysis experiments in the conditions of 320°C pyrolysis water using 72 h. The distribution of regular steranes showed great changes under pyrolysis experiments, compared with immature hydrocarbon source rocks. The relative content of the C27 regular sterane was found an increase in pyrolysis experiments with the maturity increasing. That is to say, when reaching high and over matured stage, the relatively percentage of C27, C28 and C29 regular sterane can indicate homogenization. The result shows that the C27, C28 and C29 regular sterane are uneffective to determine source type [14] [15] [16].

Although the sterane compounds have been researched widely, the relationships between the regular sterane and the thermal evolution degree have rarely been studied in nature profile. Hence, the present paper comprises a detailed study of 25 coal samples from the Tarim Basin and Ordos Basin. Through the study of the pyrolysis analysis, total organic carbon (TOC) analysis, Biomarker compounds and vitrinite reflectance and whole rock maceral analysis, the aim of this research is to explore the thermal effect on the regular sterane in hydrocarbon source rocks. In addition, it is significant for oil-source correlation and the identification of primary hydrocarbon source rocks in high-over mature, which provides the theoretical foundation for the hydrocarbon generation mechanism in coal.

2. Experimental and Samples

2.1. Samples

A total of 25 coal samples were collected from the Ordos Basin and Tarim Basin.
Ten coal samples are selected from C2y, C2j, C2b, P1t and P1s of Carboniferous to Permian in Ordos Basin, which mainly develops alluvial fan, delta, marshes and tidal flat sedimentary environment [17] [18] [19] [20]. Another coal samples are from T3h, T3t, J1y, J1k and J1q of Triassic to Jurassic, where sedimentary environment is fan delta system [19] [20]. Nineteen samples were selected for vitrinite reflectance and whole rock maceral analysis especially for this research. All coal samples were crushed into fine powder and analyzed for their contents of total organic carbon (TOC) and rock pyrolysis.

2.2. Analytical Methods

The measurement of reflectance and maceral were determined by Leica MPV-SP photomicroscope. Before the measurement, the samples were crushed to a maximum size of 1-mm. While at least 30 points were counted in every sample, then the type index (Ti) is used to calculate kerogen type indicators.

\[
Ti = \left( \text{sapropelic} \times 100 + \text{exinite} \times 50 + \text{vitrinite} \times (-75) + \text{inertinite} \times (-100) \right) / 100
\]

For total organic carbon (TOC) and rock pyrolysis, all the coal samples need to be crushed into fine powder and analyzed. However, before TOC determinations, all samples were removed by HCl treatment. The total carbon content was determined by LECO CS-2000 induction furnace. Pyrolysis was determined by Rock Eval VI made in China.

Bitumen “A” was extracted by the Soxhlet extraction for 3 days with a dichloromethane/methanol mixture (93:7 v/v). Then, the extracted bitumens were fractionated into saturated, aromatic hydrocarbons, NSOs (nitrogen, sulfur and oxygen) and asphaltenes using open column chromatography filled silica gel and the alumina. The study mainly analyzes the saturate and aromatic hydrocarbons fraction. The model of gas chromatography-mass spectrometry is HP-GC 6980/5873 MSD. And the HP-6890 GC is equipped with a HP-5MS fused silica capillary column (30 m × 0.25 mm × 0.125 μm). Helium is used as the carrier gas with a rate of 1.0 ml/min. The injector temperature is 300°C. The GC temperature is programmed to start at 50°C for 1 min; the temperature will increase to 310°C at a rate of 3°C/min with a final hold of 18 min. The scanning range is 50-550 amu.

3. Results and Discussion

3.1. Basic Geochemical Characteristics

The results of rock pyrolysis and \( R_o \) determination showed that the maturity range of coal sample from the kuqa Depression in Tarim Basin is wide. \( t_{max} \) value range from 430°C to 529°C. \( R_o \) ranges from 0.51% to 1.63% with an average value of 0.72%. In contrast the maturity of the coal samples from the Ordos Basin is relatively high. The average of \( R_o \) is 0.99%. In the whole rock maceral, \( T_i \) is an index to judge the type of parent material. The \( T_i \) index can be calculated using the relative percentage content of vitrinite, exinite, inertinite and so on. \( T_i \) values
in the selected coal sample is $-68.48$ to $-37.88$, which reveals that all coal samples are III kerogen (Table 1).

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Note: $T_1/(100a + 75b + 50c + (−75)d + (−100)e)$ represents nonfixiform organic matter, alginite, exinite, vitrinite and inertinite.
3.2. The Distribution of Sterane Compounds

In this study, the complete distribution of sterane series compounds was detected in the coal sample from Kuqa Depression and Ordos Basin. When the $t_{\text{max}}$ value is about 440˚C ($R_o = 0.7\%$), the distribution of C27 and C29 regular sterane is consistent with the typical coal measures hydrocarbon source rocks with C29 regular sterane accounting for absolute advantage. It presents asymmetrical “V” type or the “L” type (Figure 1(a)). With the thermal evolution degree increasing, the typical coal sample of C29 regular sterane relative content advantage has disappeared. On the contrary, the relative content of C27 regular sterane has a tendency of increasing (Figure 1(b)). The distributions of different maturity sterane on the same section area in Ordos basin revealed that the relative content of C27, C29 regular sterane are consistent with typical coal measures hydrocarbon source rock under the condition of low maturity ($t_{\text{max}}$ value 441˚C, $R_o$ values 0.66%). In other words, the C29 regular sterane has absolute predominance. However, with the increase of maturity, when the $t_{\text{max}}$ value reaches 499˚C, C27 regular sterane predominates, which is similar to Figure 2(b). This phenomenon is consistent with previous studies, when thermal evolution degree is higher; the C27 regular sterane relative content will gradually increase with the increasing maturation [21]. Although the samples from the same section, the distribution of C27 sterane and C29 sterane is different in different maturity. However, the distribution of C27 sterane and C29 steraneis consistency are in different parts of the section under the condition of similar maturity. Compared C27 sterane and C29 sterane, C28 sterane has no obvious change in the same profile under the condition of different maturity. That is to say, the distribution of sterane cannot be used to distinguish the hydrocarbon source rocks in the same area under the condition of different maturity.

Figure 1. The distributions of sterane in different mature coal from Kuga sag and Ordos Basin.
3.3. The Relative Content Change of Sterane Compounds

In general, aquatic organisms are rich in C_{27}ααα20R sterane, while terrigenous higher plants are rich in C_{29}ααα20R sterane. That view has been generally accepted [22]. The relationship between the relative content C_{27}, C_{28}, C_{29} regular sterane and the vitrinite reflectance $R_o$ (%) in Kuqa Depression in Tarim Basin and Ordos Basin reveals that the thermal action has influence to the C_{27}, C_{28} and C_{29} regular sterane. When the $R_o$ (%) value is less than 0.7%, the coal samples are still accounts for absolute advantage for C_{29} regular sterane. With the higher evolution degree, the relative content of C_{29} regular sterane gradually diminishes, while the C_{27} regular sterane increases. This leads to “invert” phenomenon that the content of C_{27} regular sterane is greater than the content of C_{29} regular sterane with the $R_o$ (%) values increasing continually. In the stage of mature to high mature, the relative content of C_{28} regular sterane seems to be no obvious change. Thus, in the high and over mature evolutionary stages, when using the C_{27}, C_{28} and C_{29} regular sterane to judge parent material types needs to be careful. Otherwise, the conclusions from the distribution of regular sterane may be inconsistent with the practical point in the natural profile.

3.4. The Relationship between the Sterane Compound and the Maturity Parameter $R_o$ and $t_{\text{max}}$

Previous studies illustrated the change rule of the C_{27}, C_{28} and C_{29} regulars terane compounds with the increasing maturity in simulation experiments. The change is quite outstanding especially in high or over maturity [14] [15] [16]. To further exploring the relationship between the sterane C_{27}, C_{28} and C_{29} regular sterane and the thermal action, the relationship between C_{27}/C_{29} regular sterane ratio and maturity parameters of $R_o$ (%) and $t_{\text{max}}$ (˚C) were discussed firstly (Figure 3). When $R_o$ value is 0.7% - 1.5%, the C_{27}/C_{29} regular sterane ratio has a good linear relationship with $R_o$ in the Kuqa Depression and the Ordos Basin (Figure 4(a)). Mean while, the C_{27}/C_{29} regular sterane ratio and $t_{\text{max}}$ (<500˚C) is a linear relationship, which is similar to the $R_o$ (%). That may be the thermal effect on the demethylation of C_{29} sterane obviously in the evolution stage of mature to high-mature [17] [23].
3.5. The Relationship between C$_{27}$/C$_{29}$ Ratio and Aromatics Maturity

The coal samples are at low mature to over mature stage with $t_{\text{max}}$ ranging from 432°C to 529°C. The maturity parameters of saturated hydrocarbons have reached equilibrium value; so it cannot effectively represent the maturity of samples. However, compared with the maturity parameters of saturated hydrocarbon, the maturity parameters of aromatic hydrocarbon could judge the high maturity samples. In addition to the commonly used methyl phenanthrene index MPI [24] [25], Chakhmakhchev et al. put forward dimethyl-benzothiophene maturity parameters. The works of the relationship between $R_0$ and a dimethyl-benzothiophene ratio parameter have done a lot of. And the conversion formula of $R_0$ and dimethyl-benzothiophene ratio has been put forward [26] [27]. The ratio of three methylnaphthalene TMNr = 2,3-TMN/(1,2,5-TMN + 2,3,6-TMN) were put forward [28]. And when the ratio of TMNr is greater than 0.6, it represents the high maturity [29]. In the aromatic compounds, many evaluation parameters can be used to evaluate the maturity. This present paper chose naphthalene, fluorene series compounds for research.

The C$_{27}$/C$_{29}$ regular sterane ratios and aromatic maturity parameters DMDBT and TMNr also have a good linear relationship. And the relationship is similar to $t_{\text{max}}$ and $R_0$ (Figure 5). That is to say the thermal of hydrocarbon source rocks
has distinct effect on the relative concentration distribution of regular sterane $C_{27}$, $C_{28}$ and $C_{29}$ regular sterane. So, in the same research area, the $C_{27}/C_{29}$ regular sterane ratio can be used to determine hydrocarbon source rock maturity, especially in mature-high and over mature stage of evolution.

![Figure 5](image.png)

**Figure 5.** The plot $C_{27}/C_{29}$ sterane and aromatic maturity parameters from Kuga sag and Ordos Basin.

### 3.6. The Change of Sterane in Thermal Simulation Experiment

In order to demonstrate the thermal effect on sterane distribution rules, the thermal simulation test of a coal sample had been done. Six temperature points, 200˚C, 250˚C, 300˚C, 350˚C, 400˚C, 450˚C, were chosen in the process of experiment. The results show that $C_{27}/C_{29}$ regular sterane ratio increases with the cumulative temperature rising (Figure 6). This further elucidated that the influence of the distribution of $C_{27}$ and $C_{29}$ regular sterane in the sample is objective, especially, in the high-mature stage (thermal simulative temperature >350˚C). The relationship of the absolute concentration of $C_{27}$, $C_{28}$ regular sterane and pyrolysis temperature are shown in Figure 6(b). The absolute concentration of $C_{29}$ regular sterane decrease is faster than $C_{27}$ sterane in low mature stage (thermal simulative temperature <350˚C). But when the temperature is greater than 350˚C, the $C_{27}$ regular sterane is increasing faster than $C_{29}$ regular sterane. This phenomenon proves that the $C_{27}/C_{29}$ regular sterane ratio and the degree of thermal evolution have a certain correlation.

![Figure 6](image.png)

**Figure 6.** The variation of ratios $C_{27}/C_{29}$ sterane and $C_{27}$, $C_{29}$ sterane absolute concentration with simulated temperature.
Structures determine properties in organic chemistry. It is because of the diversity of steranes compounds configuration change. Therefore, steranes compounds have high practical value in researching sources, thermal evolution and sedimentary environment of organic matter. In general, the longer chain of carbon alkane molecules is, the more will be easily broken. So the naphthene is steadier than side chain alkanes, and the more branched alkanes is prone to cracking reaction [30]. The \( C_{29} \) regular sterane adds an ethyl in \( C-24 \) place compared with the \( C_{27} \) regular sterane. Owing to hydrocarbons with different carbon number needing different chemical bond dissociation energy to fracture, it leads to the variation of \( C_{27}/C_{29} \) regular sterane ratio with the increasing thermal maturity (Table 2).

### Table 2. Bond dissociation energy related with the structure of sedimentary organic matter (Hou Dujie, et al. 2011) [31].

<table>
<thead>
<tr>
<th>C-C key</th>
<th>( \text{CH}_3-\text{CH}_3 )</th>
<th>( \text{C}_2\text{H}_5-\text{CH}_3 )</th>
<th>( \text{C}_3\text{H}_7-\text{CH}_3 )</th>
<th>( \text{C}_4\text{H}_9-\text{CH}_3 )</th>
<th>( \text{C}_3\text{H}_7-\text{C}_2\text{H}_3 )</th>
</tr>
</thead>
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<tr>
<td>Bond</td>
<td>369</td>
<td>356</td>
<td>348</td>
<td>345</td>
<td>335</td>
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<tr>
<td>dissociation</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>energy (kJ/mol)</td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
</tbody>
</table>

### 4. Conclusions

1) The steranes, especially \( C_{27}, C_{29} \) regular sterane compounds, are mainly controlled by source of parent material factor in evolution of hydrocarbon source rocks in the lower stage of development. The relative content of sterane compounds is very different in terrestrial higher plants and low aquatic algae parent material sources, so it can be served as an indicator of good source material. But on the high evolutionary stage, the relative content distribution of \( C_{27}, C_{28} \) and \( C_{29} \) regular sterane tends to be “homogenization”. In high evolution stage, therefore, it needs to be cautious to use the parameters of the relative content to determine parent material types and oil-source correlation.

2) In order to describe the relationship of the relative content of regular sterane and the thermal action, the pyrolysis experiment has been performed to show that the \( C_{27}/C_{29} \) regular sterane ratio has a good of correlation with the maturity parameter like \( R_m, t_{max} \), aromatic compounds DMDBT and TMNr. The results are similar to natural geological section, which suggests that the distribution of regular sterane will be effected by the thermal evolution.

3) To understand the characteristics of thermal evolution, the formation mechanism of the \( C_{27}/C_{29} \) regular sterane ratio with evolution degree changes is discussed by molecular structure stability. Due to the structural differences of \( C_{27} \) and \( C_{29} \) regular sterane, the demethylation effect is more apparent in \( C_{29} \) sterane than \( C_{27} \) sterane at mature to high mature evolution stage. It is the reason why the \( C_{27}/C_{29} \) regular sterane ratio rise with thermal evolution degree increasing; however, when the thermal evolution levels continue to rise, the breakage of C-C
key in branched chain makes $C_{27}/C_{29}$ regular sterane ratio invariance at high and over mature stage. Therefore, the $C_{27}/C_{29}$ regular sterane ratio may be used to distinguish hydrocarbon source rock maturity in the similar sedimentary system at high and over mature stage.

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References


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