

PRELIMINARY RESULTS OF THE SOLID-STATE C-13 NMR STUDY OF MONGOLIAN COALS: IMPLICATIONS FOR OIL AND GAS POTENTIAL AND LIQUEFACTION REACTIVITY

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ABSTRACT

Chemical structures of five coals from Mongolia were studied using solid-state C-13 NMR and oil and gas potential as well as yields of liquefaction products of the coals have been predicted. Pennsylvanian ZG, Upper Permian TT and Lower-Middle Jurassic AT-5 coals might have more potential for gas due to abundant aliphatic and aromatic CH₃ carbons. Lower-Middle Jurassic KH coal probably has more potential for oil because of its increased CH₂ content. Lower Cretaceous SO-3 coal may have more potential for gas, but significant amount of non-hydrocarbon gases could also be generated simultaneously. The prediction of yields of liquefaction product shows that ZG, TT and AT-5 and KH coals could yield similar hydrocarbon gas, oil and residue. Cretaceous SO-3 coal is predicted to give the lowest yields of oil, hydrocarbon gas and residue compared with others. KH sample has the highest oil yield due to its high content of CH₂.

Keywords: coal, petroleum potential, NMR, Mongolia

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1. Introduction

Coal is considered as important petroleum source rock especially for gas (e.g., Pashin, 2008). However, commercial oil sourced from coal have been discovered in several sedimentary basins (eg., North Sea and Hami-Turpan). It is thought that petroleum generation potential of coal is dependent on available hydrogen in coal and aliphatic chain length (Petersen and Nytoft, 2006). There are several methods used to determine petroleum potential of coal such as fluorescence and infrared (IR) spectroscopy, elemental analysis and C-13 NMR spectroscopy as well as experimental simulations including various types of pyrolysis. The bulk techniques such as elemental analysis and ¹³C NMR spectroscopy are enable a measure of the polymethylene component of the coal, which now appears to

be one of the best available approaches for determining petroleum potential (Wilkins and George, 2002).

Mongolia has huge coal resources that are hosted in Carboniferous, Permian, Jurassic and Cretaceous sedimentary rocks. The Carboniferous, Permian and Jurassic coal-bearing sequences were mainly deposited in foreland basins by compressional tectonic event, whereas Cretaceous coal measures were deposited in rift valleys caused by extensional tectonic event (Erdenetsogt et al., 2009). Petroleum potential of coal and coal-bearing sedimentary unit is not known. None of systematic studies have been completed yet. Petroleum exploration in Mongolia has been focused only on Lower Cretaceous sedimentary rocks, because known oil fields in eastern and southeastern Mongolia are sourced

from Lower Cretaceous lacustrine oil shales (Pentilla, 1994; Yamamoto et al., 1998; Johnson et al., 2003).

Geologically, western and southwestern Mongolian basins are similar to Junggar and Turpan-Hami basins in China. In these basins, number of oil fields have been discovered and produced for decades. Oil–source correlation study using biomarkers and carbon isotopes concluded that some of oils were sourced from Carboniferous and Jurassic unit hosting coal and carbonaceous shales (Difan et al., 1991; Chen et al., 2003; Xiao et al., 2010). The oil derived from coal can be distinguished easily from other oils by heavy carbon isotope compositions and high Pr/Ph ratios. Thus, it can be speculated that some oil and gas accumulations originated from coal could be discovered in western and southwestern Mongolian basins, where Carboniferous, Permian and Jurassic coals are distributed widely.

The purpose of this study is to evaluate petroleum generation potential of Mongolian coal based on bulk techniques such as elemental analysis and solid state C-13 NMR study. It should be mentioned that the prediction methods could only give initial insights into petroleum potential of Mongolian coal and resulting conclusions are preliminary. Thus, additional detailed lad analysis (organic petrology, organic geochemistry and pyrolysis) is consequential to complete the evaluation.

2.Geological setting

The coal deposits of Mongolia tend to become younger from west to east and can be subdivided into two provinces, twelve basins,

and three areas (Fig.1). Main controlling factor of coal rank is the age of coal bearing sequences (Erdenetsogt et al., 2009). Western Mongolian coal-bearing province contains mostly high rank bituminous coal in strata from Carboniferous. The basins in southern Mongolia and the western part of central Mongolia have low rank bituminous coal in strata from Permian. The northern and central Mongolian basins contain mainly Jurassic subbituminous coal, whereas the Eastern Mongolian province has Lower Cretaceous lignite.

For the present study, coal samples were collected from the mines, Zeegt (Pennsylvanian), Tavantolgoi (Upper Permian), Alagtogoo (Lower-Middle Jurassic), Khotgor (Lower-Middle Jurassic) and Shivee-Ovoo (Lower Cretaceous). Zeegt mine belongs to Mongol-Altai basin of Western Mongolian coal-bearing province. In this basin coal seams are hosted in the Middle formation of Pennsylvanian Altai Group. Tavantolgoi mine is located in South Gobi basin and coal seams are hosted in the Coal-bearing Formation of Upper Permian Tavantolgoi Group. Khotgor mine lies in Ikh Bogd basin, where Lower-Middle Jurassic unit contain coals seams. Alagtogoo and Shivee-Ovoo mines are situated in Choir-Nyalga basin of Eastern Mongolian coal-bearing province. Alagtogoo coals are related to Lower-Middle Jurassic unit, while Shivee-Ovoo coals are hosted in Khukhteeg Formation of Lower Cretaceous Zuunbayan Group. Detailed information on coal quality and the geology of the mines can be found in Erdenetsogt et al. (2009).

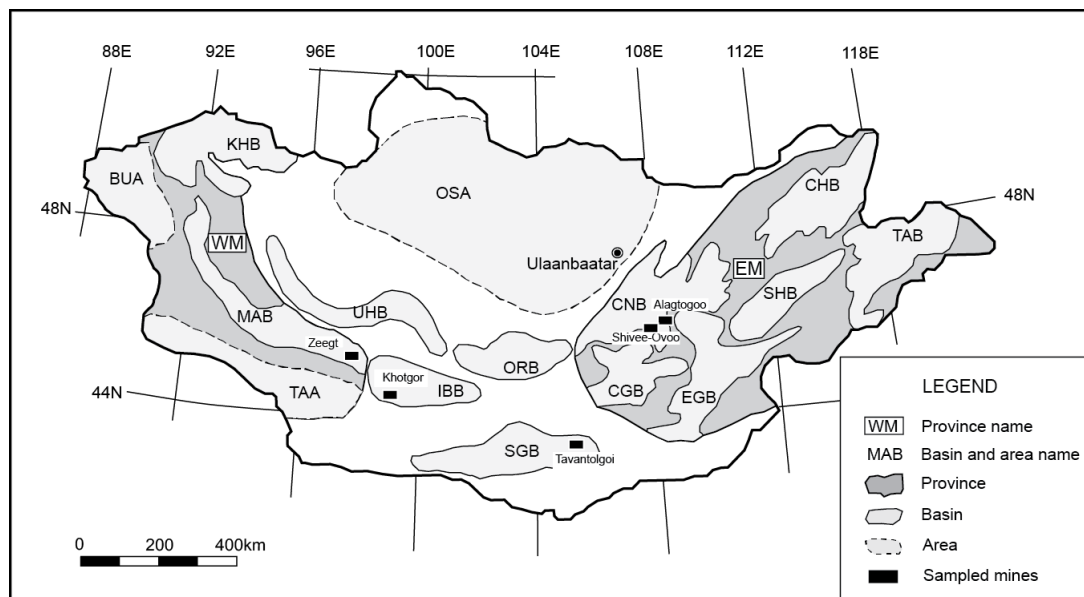


Fig. 1. Map showing sampled coal mines and locations of Mongolia coal-bearing provinces and basins (Modified from Erdenetsogt et al., 2009). Province: WM - Western Mongolian; EM - Eastern Mongolian; Basins: KHB - Kharkhiraa; MAB - Mongol-Altai; SGB - South Gobi; UHB - South Khangai; IBB - Ikh Bogd; ORB - Ongi river; CNB - Choir-Nyalga; CHB - Choibalsan; TAB - Tamsag; SHB - Sukhbaatar; EGB - East Gobi; CGB - Central Gobi basin; Areas: BUA - Bayan-Ulgii; TAA - Trans-Altai; OSA - Orkhon-Selenge.

3. Samples and methods

Five channel samples of coal were collected from fresh working faces of the Zeegt, Tavantolgoi, Alagtogoo, Khotgor and Shivee-Ovoo mines (Fig. 1). Samples were to pass through a 70 mesh sieve and pretreated with hydrochloric acid to remove carbonate minerals. The elemental analysis (C, H, N, total S, and O) was performed at the National Center for Inter-University Research Facilities (NCIRF) at Seoul National University, using EA 1110 and EA 1112 analysers (CE instruments). The molecular structures of coal samples were determined using solid-state C-13 NMR at NCIFR. The experiments were performed using a Bruker Avance II 500 NMR spectrometer at a carbon frequency of 125.77 MHz and a proton frequency of 500.12 MHz. z. Dry, powdered samples were packed into a 4 mm zirconia rotor with a Kel-F cap. The {H-1} C-13 CP/MAS spectra were recorded at a

spinning speed of 10 KHz using a triple resonance probe. The measurement conditions were as follows: the contact time was 3 ms, with a recycle delay of 1 s and a scan number of 5120.

The spinning speed of 10 KHz was not fast enough to remove the spinning side bands (SSB), which appeared in the spectra. Thus, SSB correction was completed based on the deconvolution of the spectra. The bands centered at around 40 ppm, 63 ppm, 205 ppm and 220 ppm were assigned to SSB and their areas were excluded from the calculation of the relative percentages of other bands. It should be noted that the relative percentages of the ranges between 90–120 ppm and 60–90 ppm have relatively low accuracy for SO-3 and KH sample, because low field SSB from the resonance at 32 ppm and the high field SSB from the resonance at 143 ppm were

completely overlapped by the resonances at around 113 ppm and 63 ppm, respectively.

4. Results and discussion

4.1. Elemental composition of samples and reliability of NMR data

During the coalification process, the carbon content increases, whereas the oxygen content decreases progressively (Petersen et al., 2008). In contrast, the hydrogen content remains constant up to the rank of medium volatile bituminous coal and then decreases up to anthracite (Diessel, 1992). Hence, elemental composition and H/C and O/C ratios can be used as rank parameters.

The C content of the samples coals ranges from 70.0 to 85.6 wt.% and the O content ranges from 24.7 to 5.9 wt.%. The H content varies between 4.1 and 5.5 wt.%. The N and S contents range from 1.0 to 2.6 wt.% and from 0.1 to 1.0 wt.%, respectively. The low contents of S indicate a non-marine influence. H/C and O/C ratios of ZG and TT samples are similar, indicating similar coal rank. H/C ratios of AT-5 and KH samples are similar. However, O/C ratios of the samples are quite distinct. SO-3 sample has H/C ratio of 0.82 and O/C ratio of 0.25.

Fig. 2 shows that the coal rank of ZG, TT and AT-5 samples are similar, at bituminous rank. However, TT is slightly higher than

others (Table 1). Without doubt, SO-3 sample is lignite because of its high H/C and O/C ratios. Interestingly, H/C ratio of KH sample is similar to that of AT-5 sample, but O/C ratio is within the range of lignite. Thus, it is likely that increased oxygen content of KH sample is due to increased amount of aliphatic materials with high O content that were incorporated in the sample during burial, which were preserved well (see discussion below).

To test the reliability of the NMR data, elemental compositions of C, H, and (O+N) were estimated from the NMR spectra according to the method described in Mao et al. (2000). Fig. 3 shows the %C and %(O+N) estimated from the quantification of CP/MAS NMR spectra and those from ultimate analysis. The dashed lines represent a 1:1 relationship. The result indicates that the element fraction obtained from NMR spectra is consistent with the ultimate analysis, especially for the samples having high H/C and low O/C atomic ratios. It is previously known that the precision of NMR quantification decreases with increase in oxygen contents (Yoshida et al., 2002). Mao et al. (2000) also noted that systematically high H content in the sample estimated using direct polarization NMR data due to the overestimation of the H content of some of the carbon types.

Table 1. Elemental analysis data of samples with their ages

Sample #	Age	C	H	O	N	S	H/C	O/C
ZG	Pennsylvanian	82.7	5.5	9.0	2.6	0.3	0.79	0.08
TT	Upper Permian	85.6	5.5	5.9	2.1	0.8	0.77	0.05
AT-5	Lower-Middle Jurassic	83.7	4.8	8.6	1.8	1.0	0.69	0.08
KH	Lower-Middle Jurassic	70.0	4.1	24.7	1.0	0.1	0.71	0.26
SO-3	Lower Cretaceous	70.4	4.9	23.4	1.0	0.4	0.82	0.25

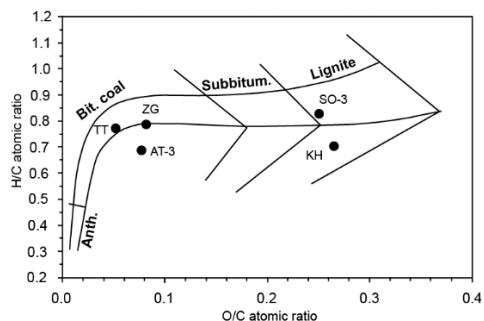


Fig. 2. Plots of atomic H/C vs. O/C ratios for the samples. Boundary between coal rank is adopted from Suggate (2000). More detailed explanation could be found in Suggate (2000).

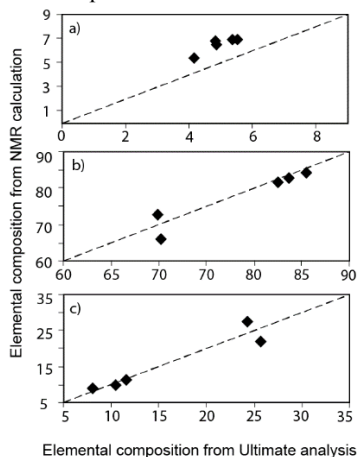


Fig. 3. The comparison of elemental composition from elemental analysis and NMR calculations; (a) hydrogen, %; (b) carbon, %; (c) (O+N), %. Dashed line represent a 1:1 relationship.

4.2.C-13 CP/MAS NMR peak assignments

NMR spectra were interpreted based on previous studies of humic soil, insoluble organic matter, cellulose, lignin, peat, coal and coal yields (Hatcher, 1988; Yoshida et al., 2002; Almendros et al., 2003; Erdenetsogt et al., 2010). The C-13 CP/MAS NMR spectra of the coal samples studied here are shown in Fig. 4. The spectrum of Lower Cretaceous SO-3 sample is distinguishable from others, because lower rank coals (lignite) contain relatively complex oxygen-functional groups that are eliminated at around subbituminous rank. The following peak assignments are for the NMR spectrum of sample SO-3.

The spectra of coals can generally be divided into two main chemical regions: aliphatic carbons (0–90 ppm) and aromatic carbons (90–220 ppm, including carbonyl/carboxyl and phenolic groups). In the aliphatic carbon region, a peak of 30–32 ppm originates from methylene carbons in aliphatic chains. A small shoulder at ~14 ppm originates from terminal methyl groups of aliphatic chain. A shoulder at ~55 ppm is assignable to methoxyl carbon. A peak at 74 ppm is aliphatic alcohol and ether carbon with contribution from residual carbohydrate carbon. In the aromatic carbon region, peaks at 115 and 125 ppm are assigned to protonated aromatic carbon. The peak at around 115 ppm is characteristic of protonated aromatic carbon

ortho or para to aromatic-O carbon. The peak at 125 ppm is protonated aromatic carbon at least two bonds away from an oxygen-substituted aromatic carbon. A peak at ~144 arises from O-substituted aromatic carbon of the dihydric (or methoxy) phenols such as catechol. Peaks at 175 and 195 ppm are carboxyl and carbonyl carbons, respectively.

The higher rank samples (e.g., TT) have a discernible peak at 20 ppm that is from methyl groups directly attached to aromatic ring. In addition, shoulders at 140 ppm and 153 ppm can be assigned to carbon-substituted aromatic carbons and monohydric phenolic carbons, respectively.

Based on the results of elemental analysis and NMR study, one can say that SO-3 sample is at the end of lignite rank, because lignite contains the various types of oxygen-containing functional groups (Petersen et al., 2008). In addition, at the beginning of subbituminous rank, methoxyl (~55 ppm), protonated aromatic (115 ppm), dihydroxy (or methoxy) phenol (144 ppm) and carbonyl (195 ppm) are decreased significantly (e.g., Erdenetsogt et al., 2010). For SO-3 sample, the peaks are identifiable, which indicates that the sample is at the end of lignite rank. In the middle of subbituminous coal rank, all of

oxygen containing function groups are removed from coal except hydroxyl groups of phenolic carbon (e.g., Hatcher and Clifford, 1997). The three spectra of AT, TT and ZG samples are similar and there are no peaks from oxygen containing groups except the shoulders at 153 ppm. This is an indication of presence of phenolic carbon. Another distinguishable feature is a peak at 20 ppm that is from pendant methyl groups. The groups are abundant at bituminous rank (Obeng and Stock, 1996).

KH sample is quite distinct from others. According to EA results, the sample falls into lignite rank (Fig. 2), but NMR spectra of the sample does not match with that of lignite. As mentioned above, lignite spectra (e.g., SO-3) have discernible peaks at 55 ppm, 115 ppm, 144 ppm and 195 ppm that are absent in the KH spectra. Moreover, shoulders at 20 ppm and 153 ppm are observed from KH spectra. Thus, it is more likely that the rank of KH sample is higher than subbituminous rank. The sharp peak at 30 ppm and discernible peaks at 72 ppm and 86 ppm are most likely from aliphatic materials that are incorporated in the sample during the burial. Due to high content of O-substituted aliphatic carbons (72 ppm and 86 ppm), O/C atomic ratio is elevated compared with another Jurassic sample, AT-5.

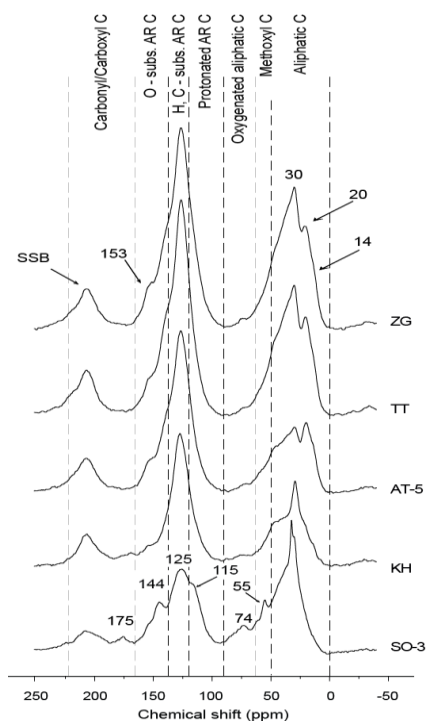


Fig. 4. The solid state C-13 NMR spectra of the samples with labels as ppm. The relative percent of carbon types are in Table 2.

4.3. Oil and gas potential

A wide range of geochemical technique is used for the assessment of petroleum generation potential. However, there is no single parameter that is universally accepted as an accurate measure of the petroleum generation (Wilkins and George, 2002). In this subchapter, the results of two techniques applicable for bulk coal samples are compiled.

4.3.1. EA analysis

Coal is classified as Type III kerogen that has H/C ratio lower than 0.8 (e.g., Vandenbroucke and Largeau, 2007). Type III kerogen is characterized predominantly by aromatic structures, heteroatomic ketones, and carboxylic acid groups and contains a relatively minor proportion of aliphatic and alicyclic compounds (Pashin, 2008). Due to its low content of H, type II kerogen is recognized as gas prone source. Some Jurassic and Tertiary coal have vitrinite, containing more

than 5.5% H. These coals having perhydrous vitrinite are suggested to be liquid hydrocarbon source (Wilkins and George, 2002, references therein).

The H contents of coal samples range from 4.1 to 5.5 wt.%, suggesting that the coals are orthohydrous and subhydrous coals (Fig. 5). Carboniferous ZG and Permian TT coals have relatively elevated H contents (~5.5 wt. %), indicating that the coals have more hydrocarbon potential compared with others.

Saxby (1980) found systematic relationship between the elemental chemical composition of coal and oil yield based on open-system pyrolysis experiments. The relationship can be expressed as

$$\% \text{ oil (wt.\%; dry; mineral free)} = 66.7 \text{ H/C} - 57.0 \text{ O/C} - 33.3 \quad (\text{Eq. 1}).$$

It is known that increased O contents has negative effect on oil generation from coal. For example, Boudou et al (1994) found that

decarboxylation and dihydroxylation of lignite and bituminous vitrain before pyrolysis resulted in a substantial increase and acceleration of oil formation. In addition, Longbottom et al. (2016) revealed that O-substituted aromatic carbons (Ar-C) have large negative effect on hydrocarbon generation.

Oil yield from the coal samples have been predicted by using the relationship and could be between 8.2 wt.% to 15.3 wt.% (Table 3, Fig.6). The oil yields of Carboniferous ZG and

Permian TT coals have been predicted to be ~15 wt.%, while that of Jurassic AT-5 has been predicted to be 8.2 wt.%. Main reason for lowered oil yield for AT-5 coal is H content. ZG and TT samples have the high H contents, whereas AT-5 sample has lower H content (Table 1). The oil yields of Jurassic KH and Cretaceous SO-3 samples have not been estimated, because Eq.1 is valid only for coals having O/C atomic ratio less than 0.15.

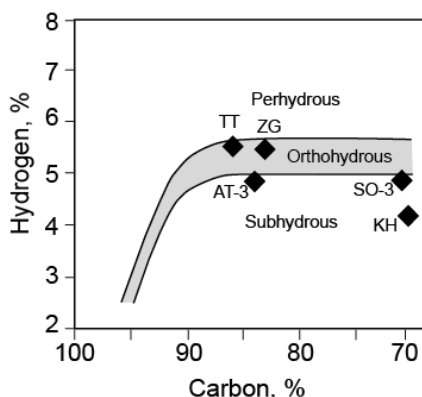


Fig. 5. Plots of the samples on simplified Seyler chart with the compositional fields of orthohydrous, perhydrous and subhydrous coals. Diamonds represent the samples. After Diessel (1992).

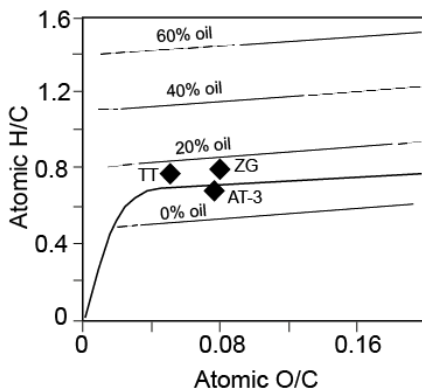


Fig. 6. Plots of samples on atomic H/C vs. O/C diagram showing vitrinite maturation line and calculated oil yields for slow pyrolysis under geological conditions (Saxby, 1980)

4.3.2. C-13 NMR spectroscopy

The distributions of carbon types of samples, based on deconvolution of the NMR

spectra, are shown in Table 2. These are subdivided into two main groups: aliphatic and aromatic carbon types. The carbon type distributions of Carboniferous ZG, Permian TT

and Jurassic AT-5 samples are broadly similar. O-substituted aliphatic carbons and carbonyl/carboxyl carbons are absent and the contents of other carbon types including H-, C- and O-substituted aromatic carbons as well as aliphatic carbons are almost identical (Fig. 7). Among them, TT sample has the lowest H-substituted aromatic carbon and the highest C-substituted aromatic carbon indicating higher coalification rank. Another interesting feature is that samples, ZG, TT and AT-5, have relatively high contents of terminal aliphatic and aryl CH₃ (peaks at 14 ppm and 20 ppm). Demethylation of the methyl groups is considered as the main pathway of the generation of CH₄ (Obeng and Stock, 1996; Cramer, 2004). SO-3 sample has the most varied O-containing carbon types and the lower aliphatic and aromatic carbon types that is the characteristics of lower rank coal. SO-3 sample has 5% of OCH₃, which could generate CH₄ at lower coalification stage (Cramer, 2004). KH sample is again distinct from others. The sample has higher O-containing aliphatic and aromatic carbons as well as methylene. The methylene and O containing aliphatic carbons are probably derived from liptinitic materials.

Based on pyrolysis and C-13 NMR study, Qin et al. (1991) found that aliphatic methylene and methine carbons directly related to oil yield, while aromatic carbons contribute little to oil and gas formation. They classified methylene and methane as oil prone carbons (fo; 25-45 ppm) and other aliphatic carbons together with carbonyl and carboxyl carbons as gas prone carbons (fg; 0-25 ppm, 45-90 ppm and 165-220 ppm). Aromatic carbons were classified as inert carbons (fa; 90-165 ppm). Carboniferous ZG, Permian TT and Jurassic AT-5 samples have similar inert (av. 62.3 wt.%), gas (av. 10.6 wt. %) and oil prone (av. 27.1 wt.%) carbon fractions (Table 2). Cretaceous SO-3 sample has the highest gas

prone carbon content (27.9 wt. %) and the lowest inert carbon content (48.9 wt.%). Jurassic KH sample has the highest oil prone carbon content (33.9 wt.%). The high fg of SO-3 is due to its high contents of O-containing aliphatic and carbonyl/carboxyl carbons, whereas high fo of KH is largely dependent on its increased amount of methylene (30 ppm). Overall, these data indicate that all samples have relatively good oil and gas potential. However, the potential depends on expulsion efficiency (Wilkins and George, 2002).

As mentioned above, O-containing functional groups have negative or positive influence on oil and gas generations. Together with other aromatic carbons, phenolic carbons have large negative impact on hydrocarbon generation (Boudou et al., 1994; Longbottom et al., 2016). All samples except KH have similar O-substituted aromatic carbons (~8.8%). KH sample have much higher O-Ar carbon (19.6 %) that could have more suppression on hydrocarbon generation compared with other coals. However, such high contents of phenolic carbons are not common for the coal at this rank. Further detailed investigations for the distribution of carbon types of KH sample are required.

Overall, Pennsylvanian ZG, upper Permian TT and Lower-Middle Jurassic AT-5 coals might have more potential for gas due to abundant aliphatic and aromatic CH₃ carbons. The three coals have highest inert carbon fractions. Lower-Middle Jurassic KH coal probably has more potential for oil because of its increased methylene content. The coal having the higher proportion of CH₂ is always considered as potential source rock for oil (Petersen and Nytoft, 2006). Lower Cretaceous SO-3 coal may have more potential for gas, but significant amount of non-hydrocarbon gases could also be generated simultaneously. SO-3 coal has lowest inert fraction.

Table 2. Integrated intensity distribution of the carbon types of samples as well as oil, gas and inert fractions
(All values are in %)

Sample #	CH ₃ -Al	CH ₃ -Ar	CH ₂	CH ₃ O	CH ₂ O	ArC-H	ArC-C	ArC-O	CO, COOH	fg	fo	fa
ZG	6.4	4.7	27.1	0.0	0.0	9.1	42.8	9.9	0.0	11.0	27.1	61.9
TT	5.4	6.4	25.3	0.0	0.0	7.5	47.8	7.6	0.0	11.7	25.3	63.0
AT-5	5.8	3.4	28.9	0.0	0.0	10.8	42.3	8.9	0.0	9.2	28.9	62.0
KH	1.7	2.2	33.9	0.0	2.8	6.7	32.9	19.6	0.0	6.8	33.9	59.3
SO-3	1.7	4.2	23.2	4.9	11.9	4.3	35.8	8.8	5.2	27.9	23.2	48.9

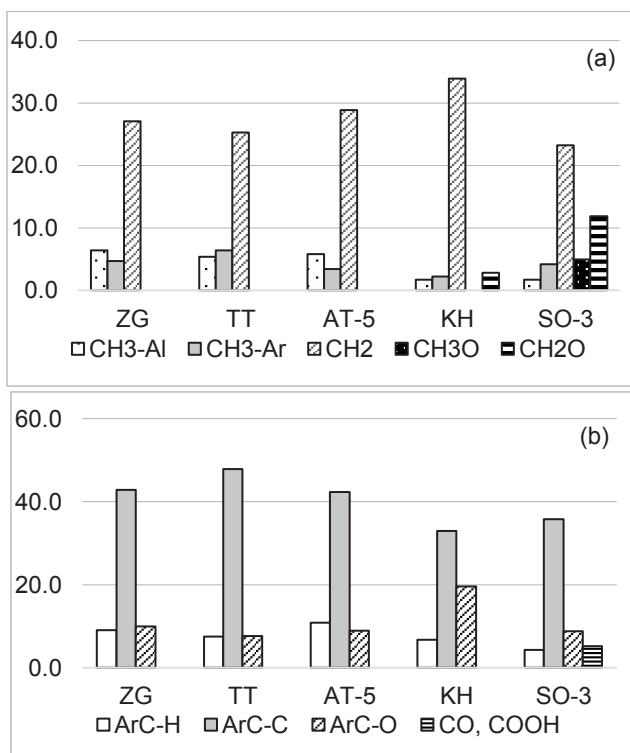


Fig. 7. Distribution of carbon types; (a)aliphatic carbons and (b)aromatic and carboxyl/carbonyl carbons.

4.4. Prediction of coal liquefaction reactivity

Yoshida et al. (2002) found a good relationship between structural data derived from solid state C-13 NMR spectra and liquefaction data of coals. They concluded that the yields of liquefaction products could be predicted from C-13 NMR spectral data of

coal. The liquefaction data of coal was obtained by use of 1 t/d NEDOL process support unit (PSU) and 150t/d NEDOL pilot plant (PP). Seven kinds of coal from five different countries were used for liquefaction tests. Correlation equations for prediction of liquefaction products (hydrocarbon gas, CO_x gas, water, oil and residue) are shown below:

$$\text{Hydrocarbon gas (HC wt.\%)} = 0.33 (\text{CH}_2 + \text{CH}_3) \% + 6.15 \quad (\text{Eq.2})$$

$$\text{CO}_x \text{ gas (O}_{\text{CO}_x} \text{ wt.\%)} = 1.43 (\text{CO} + \text{COOH}) \% - 1.45 \quad (\text{Eq.3})$$

$$\text{Water (O}_{\text{H}_2\text{O}} \text{ wt.\%)} = 2.03 (\text{AR-O} + \text{OCH}_3) \% - 10.84 \quad (\text{Eq.4})$$

$$\text{Oil (wt\%)} = 0.86 \text{ CH}_2\% + 27.5 \quad (\text{Eq.5})$$

$$\text{Residue (wt.\%)} = 122.0 \text{fa} - 49.2 \quad (\text{Eq.6})$$

By using the correlations, liquefaction products of the samples have been predicted (Table 3). The results show that Carboniferous ZG, Permian TT and Jurassic AT-5 and KH samples could yield similar hydrocarbon gas, oil and residue. Cretaceous SO-3 could yield lower oil, hydrocarbon gas and residue compared with others. KH sample has the highest oil yield, 56.7% due to its high content of CH₂. Water contents of KH and SO-3 samples are 29 wt.% and 17 wt.%, respectively. This is because of the high contents of the phenolic carbons of KH sample and the oxygenated aliphatic carbons of SO-3. Residue

of SO-3 sample is lower - 10.4%, while that of other samples are relatively higher, ranging from 23.1 wt.% to 27.6 wt.%. The sample SO-3 is lignite, of which aromaticity is lower than others. Unrealistic yields in these prediction are the yields of CO_x. For higher rank coal samples, CO_x contents were estimated to be negative value due to the absence of carboxyl/carbonyl carbons in the sample. It is clear that during the real liquefaction process, CO_x is generated largely. This indicate that the prediction equation for CO_x content is required a revision

Table 3. Predicted oil yield and liquefaction products

Sample	Oil yield prediction (Saxby 1980)	Coal liquefaction prediction (Yoshida et al., 2002)				
		HC gas	CO _x	H ₂ O	Oil	Residue
ZG	14.5	18.7	-	9.4	50.8	26.3
TT	15.3	18.4	-	4.7	49.2	27.6
AT-5	8.2	18.7	-	7.3	52.3	26.4
KH	n.d.	18.7	-	29.0	56.7	23.1
SO-3	n.d.	15.7	6.0	17.0	47.5	10.4

Note: n.d.-not determined

5. Conclusions

Chemical structures of five coals from Mongolia were studied using solid-state C-13 NMR. The ranks of coals range from lignite (SO-3) to bituminous coal (ZG, TT and AT-5). Based on the results of NMR study and EA, oil and gas potential as well as yields of liquefaction products of the coals have been predicted.

Pennsylvanian ZG, Upper Permian TT and Lower-Middle Jurassic AT-5 coals might have more potential for gas due to abundant aliphatic and aromatic CH₃ carbons. Demethylation of CH₃ is main pathway for CH₄ generation at bituminous rank. Lower-Middle Jurassic KH coal probably has more

potential for oil because of its increased CH₂ content. It is thought that oil prone coal has the elevated contents of CH₂. Lower Cretaceous SO-3 coal may have more potential for gas, but significant amount of non-hydrocarbon gases could also be generated simultaneously.

The prediction of yields of liquefaction product shows that Carboniferous ZG, Permian TT and Jurassic AT-5 and KH samples could yield similar hydrocarbon gas, oil and residue. Cretaceous SO-3 could yield lower oil, hydrocarbon gas and residue compared with others. KH sample has the highest oil yield due to its high content of CH₂.

It should be noted that this is preliminary results of oil and gas potential of Mongolian

coal. In the future, comprehensive studies (organic petrology, organic geochemistry and pyrolysis) should be completed in order to evaluate the oil and gas generation potential of Mongolian coal. This kind of systematic survey is vital for not only Mongolian coal geology, but also the source rock evaluation of continental coal-bearing units that are widely distributed in Asian interior.

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