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CHARACTERISTICS OF EXTRACTS AND COKING ABILITY OF DONETSK COALS**L. Butuzova¹, A. Bechtel², Sh. Shakir¹, G. Butuzov¹**¹ Donetsk National Technical University² Department of Applied Geosciences & Geophysics, University of Leoben, Austria**Abstract**

The pairs of the isometamorphic Donetsk coking (~83-88 % C^{daf}) and non-coking (~76-79 % C^{daf}) coals formed under reductive (RC) and less reductive conditions (LRC) have been studied. A comparative study of extracts and thermal destruction process of RC and LRC has been carried out. The yield and composition of soluble fractions of coal organic matter was characterized by liquid chromatography and Gas-Chromatography-Mass-Spectrometry (GC-MS) methods. Obtained results show significant differences in the yield and composition of the hydrocarbons for the coking and non-coking coals. The relationship between the hydrocarbon composition of coals and their depositional environment was described. The chemical characteristics of coals deposited under different redox were outlined. It is established that the yield of alkylated biphenyls correlates with the important technological characteristic of coals such as yield of semi coking liquid products.

Keywords: sulfur coals, structure, biomarkers, gas chromatography-mass-spectrometry

1. Introduction

Coal facies can be describe as alluvial and marine where deposits are laid down in swamp lakes, ponds, rivers or seas. Coals formed under reduced (RC) and low-reduced (LRC) conditions during early diagenesis have a special property (Marinov at al, 2000; Bechtel et al. 2002; Mat-senko 1983; Butuzova et al., 2002, 2005a,b,c). Marine-influenced bituminous coals (reduced coals) haven't been studied enough though the high sulfur content is a serious problem for its utilisation.

The Donetsk coal basin is a classical example of carboniferous coal accumulation in mul-tifacial depositional environments, i.e. alluvial and marine. Thus samples of Donetsk coals can be used for the examination of influence of depositional setting on their composition and properties.

Previous investigations indicate that the organic sulfur content is a major indicator for dis-tinguishing between RC and LRC coals, which correlated with dibenzothiophene / phenanthrene ratio, with the content of hopanes and the $\delta^{13}\text{C}$ values in coal extracts (Bechtel et al. 2002). The dependence of the coal structure and reactivity on sulfur content is fairly strong (Butuzova et al., 2009a,b). The reactions of -S- and -O- containing groups affect the thermodestruction processes resulting in variations in the yield and composition of liquid, solid and gaseous products and the degree of coal organic matter (COM) conversion. The semi-coking of low rank RC samples pro-duce a substantially higher yield of tar and higher content of aliphatic hydrocarbons in semi-coking gas and tar than LRC (Butuzova et al., 2009b; Butuzova et al., 2005b). So, low rank RC may be a suitable raw material for oil generation (Petersen, Nytoft, 2006).

The statistical dependence between the organic sulfur content and the main classification parameter - volatile matter yield has been found for the Donetsk low-rank coals, with the correla-tion coefficients being $R^2 = 0.89-0.95$ (Butuzova et al. 2005, b). Some structural parameters of coals correlate with S_o^{daf} .

A high reactivity of reduced coals in coking and lacing processes has been described (Bu-tuzova et al. 2005a,b; Safin et al. 2009). But the theoretical aspects of chemistry of the coal thermal destruction processes have not been sufficiently investigated to allow the prediction of the results of coal processing on the basis of coal characteristics.

The aim of the present paper is a detailed comparative study of the geochemical character-istics for non-coking and coking coals which are the main raw material for coking industry and elucidation of the connection between yield, composition of extractable organic matter and sulfur content using organic geochemical, thermal, chemical, and petrographic methods.

2. Experiment

2.1. Samples

The samples studied include four pairs ("RC-LRC") of non-coking coals of D-Grade and coking coals of J-Grade, according to Ukrainian classification (Table 1). Their geological age is Middle Carboniferous. They have uniform petrographic composition: 80-89% of vitrinite, 3-8% of liptinite, 5-14% of intertinite. Each pair of samples of the low-reduced and reduced coals was collected from neighbouring coal seams (separated by less than 100 m). Limestone layers at the top of the coal seams and finely crystalline pyrite presence were reliable signs of a reduced type of Donetsk coals. In addition, the content of microlithotypes with finely dispersed pyrite (carbopyrite) was identified. It is also an indicator of reduced and low-reduced type of coals (Matsenko, 1983).

To determine the most expedient way of sulfur coals technological employment it is important to establish the relationship between various types of the sulfur compounds in coal organic matter (COM) and the basic properties of solid fuels. Statistical methods are applied to the data set derived from the analysis permitting a quantitative description of the effect of the contribution of sulfur into the formation of coal properties.

The statistical analysis was performed using the Microsoft Excel and Origin 6.1 software package. Qualitative characteristics of the Donetsk Basin coal seams given in the reference book on the quality of various rank coals and anthracites of the Donetsk and Lviv-Volyn Basins (Catalogue 1972) were used as the data base. All the samples of the Middle Carboniferous J-Grade coals mentioned in the reference book have been selected. From this selection 100 samples are characterized by proximate and ultimate analysis for the total sulfur content (of the seam sample), the volatile matter yield (wt %), the plastometric indicator (i.e. y), the elemental composition (i.e. the carbon, hydrogen, sulfur and oxygen contents) and the atomic ratios of the individual elements to carbon determination.

The proximate, ultimate and petrographic analysis of samples, including total sulfur (S_t), organic (S_o), pyrite (S_p) and sulphate (S_s) were determined by using standard methods (State Standards 9414.3-93, 12113-94, 27314-91, 11022-95, 8606-93, 6382-91, 2408.1-95, 2408.3-95). The total organic carbon content was measured on a Leco carbon analyser on the samples pretreated with concentrated hydrochloric acid and calculated on a dry and ash-free basis (C^{daf} , wt % of the sample; Table 1).

Table 1. Characteristics of initial coal

№	Coal Grade	Coal mine (deposit), coal seam	Type	Proximate analyses (wt%)							Ultimate analyses, daf (wt%)			
				W ^a	A ^d	V ^{daf}	Y _{MM}	S _t ^d	S _s ^d	S _p ^d	C	H	O+N	S _{org}
1	D	Cheluskintsev, l ₄	LRC	0.8	2.4	35.6	-	2.17	0.04	0.11	79.3	4.94	13.7	2.02
2	D	Trudovskaya, l ₄	LRC	1.0	1.6	37.3	-	1.05	0.01	0.08	78.4	4.95	15.8	0.96
3	J	Gagarina, m ³	LRC	1.2	3.7	28.7	22	0.70	0.06	0.03	87.4	5.1	6.9	0.6
4	J	Zasyad'ko, l ₄	LRC	1.4	2.6	31.7	16	1.09	0.01	0.24	87.8	5.16	7.0	0.8
1 ¹	D	Ukraine, k ₈	RC	1.5	9.9	41.8	-	2.87	0.11	0.80	77.9	5.30	14.6	2.17
2 ¹	D	Trudovskaya, k ₈	RC	0.9	4.6	46.2	-	5.85	0.05	0.71	76.1	5.43	13.7	5.33
3 ¹	J	Gagarina, m ₄ ⁰	RC	0.8	12.2	35.6	32	3.75	0.05	2.41	83.6	4.9	10.0	1.3
4 ¹	J	Zasyad'ko, l ₄	RC	0.8	2.7	31.7	27	2.81	0.02	1.14	87.3	5.23	7.2	1.7

The analysis of the coal dichloromethane extracts by the medium-pressure liquid chromatography and high resolution gas chromatography was carried out by the technique described earlier (Bechtel et al. 2002).

3. Results and discussion

Data from the proximate and ultimate analyses of coals are given in Table 1. Samples of reduced coals are distinguished by higher S_o^d , S_p^d and total sulfur contents, higher H/C ratio and yields of volatile matter than low reduced coals corresponded to the same degree of coalification. For coals under study organic sulphur S_o^d is the main form of sulphur.

Petrographic composition of investigated coals is uniform enough with predominant presence of vitrinite. The lower value of vitrinite reflectance (R_m^0) and higher content of lithotypes with finely crystalline pyrite are recorded in RC samples.

The results of statistical analysis are given in Table 2. These data show that the R^2 values between the volatile matter yield and the atomic ratio S_o^{daf}/C^{daf} fall down up to 0.35 for the middle rank coal. At the same time the correlation between S_o^{daf}/C^{daf} and thickness of plastic layer (y) appears at this coal rank.

Then some groups of samples with different ranges of O^{daf}/C^{daf} values were selected (Table 2). The correlation coefficients within these groups increase when the interval of O^{daf}/C^{daf} is narrowing down, i.e. at a more distinct registration of the coal rank.

Table 2. The variation of correlation coefficients value in different intervals of O^{daf}/C^{daf} for the G-grade coals: atomic S_o^{daf}/C^{daf} ratio versus volatile matter yield (R_{V-S}) and versus thickness of plastic layer (R_{Y-S}).

Number of coal	intervals of O^{daf}/C^{daf}	R_{V-S}	R_{Y-S}
100	0.026-0.120	0.35*	0.64*
91	0.042-0.093	0.43*	0.62*
62	0.050-0.080	0.59*	0.60*
43	0.055-0.075	0.58*	0.61*
27	0.060-0.070	0.55*	0.58*
22	0.050-0.060	0.72*	0.56*
24	0.070-0.080	0.61*	0.68*

Table 3. The variation of correlation coefficients value versus coalification degree

Number of coal	Interval O/C	R_{V-S}	R_{Y-S}
8	0.10-0.09	0.66	0.83
19	0.09-0.08	0.55	0.67
19	0.08-0.07	0.61	0.64
22	0.07-0.06	0.52	0.59
21	0.06-0.05	0.72	0.56
9	0.05-0.04	0.36	-0.15

The influence of coalification degree on the above correlations can be seen also from Table 3, where the range of O^{daf}/C^{daf} ratio changes in the interval 0.01 for each group of selected samples. The results show that the correlation coefficient for R_{Y-S} worsen significantly for coals having O^{daf}/C^{daf} ratio less than 0.1 and for R_{V-S} value the same worsening appears for coals having O^{daf}/C^{daf} ratio less than 0.05.

An apparent correlation between the S_o^{daf}/C^{daf} ratio and thickness of plastic layer reflects the effect of sulfur on coal caking ability.

As can be seen from Table 4, the extracts obtained from RC coals are characterized by a higher content of polar heterocompounds, as well as aromatic hydrocarbons, which corresponds

to their high coking ability. The yield of dichloromethane extract is higher for RC in comparison with LRC, which is indicating an increased solubility of organic matter from reduced samples.

Table 4. Concentrations ($\mu\text{g/g C}^{\text{daf}}$) and their ratio of specific components in the aliphatic and aromatic fractions

Coals Grade								
Compounds	1	2	1 ¹	2 ¹	3	J	3 ¹	4 ¹
Sum (n-Alkanes)	60.6	27.93	36.54	73.36	8.95	4.60	8.58	8.89
n-C ₁₅₋₁₉ / C ₁₅₋₃₅	0.12	0.11	0.09	0.19	0.32	0.67	0.43	0.50
n-C ₂₁₋₂₅ /n-C ₁₅₋₃₅	0.27	0.24	0.20	0.16	0.38	0.14	0.31	0.21
n-C ₂₇₋₃₁ /n-C ₁₅₋₃₅	0.42	0.48	0.50	0.43	0.15	0.10	0.13	0.17
CPI ^a	1.43	1.42	1.22	1.13	1.24	1.15	1.20	1.28
Pr ^b / n-C ₁₇	5.58	6.82	6.40	2.34	0.88	0.90	0.71	0.70
Ph ^c / n-C ₁₈	1.10	1.41	1.71	0.93	0.40	0.78	0.57	0.82
Pr/Ph	5.64	5.45	4.24	2.99	2.73	2.12	1.78	1.46
C ₂₇ Steranes	0.92	0.58	5.73	10.36	0.10	0.09	0.75	0.41
C ₂₈ Steranes	0.73	0.44	3.76	7.53	0.09	0.05	0.35	0.11
C ₂₉ Steranes	3.28	2.47	5.81	17.19	0.23	0.21	1.20	0.76
Diasteranes	1.36	0.75	5.73	13.35	0.00	0.00	0.00	0.00
4 α Methylsteranes	2.90	1.26	0.64	7.34	0.00	0.00	0.00	0.00
20S/(20S+20R) C ₂₉ Steranes	0.41	0.36	0.48	0.39	0.54	0.52	0.56	0.52
$\alpha\beta$ Hopanes	26.93	16.93	25.57	69.23	0.57	0.47	1.85	1.24
$\beta\alpha$ Hopanes	10.46	7.23	8.17	27.54	0.22	0.09	0.70	0.56
Hopanes	37.80	24.52	34.22	97.16	0.79	0.56	2.55	1.80
22S/(22S+22R) C ₃₁ Hopanes	0.6	0.52	0.57	0.48	0.59	0.57	0.61	0.59
Steranes / Hopanes	0.24	0.22	0.63	0.57	0.54	0.40	0.65	1.06
Diterpenoids Saturated	3.87	4.76	4.87	8.04	0.53	0.23	0.42	0.17
Aromatic Diterpenoids	8.88	17.24	26.94	29.34	2.12	1.41	1.61	2.77
Diterpenoids(Sat.+Aromatic)	12.75	22.00	31.81	37.38	2.64	1.63	2.03	2.95
Sat-/ Arom- Diterpenoids	0.44	0.28	0.18	0.27	0.25	0.16	0.26	0.06
Tri(Tri+Mono) Arom. Steroids	0.55	0.61	0.64	0.47	0.00	0.00	0.00	0.00
Naphthalene	1.60	1.34	4.26	1.17	0.15	1.27	0.22	0.40
Methylnaphthalenes	18.39	15.08	33.25	11.22	4.90	6.97	2.62	12.53
Dimethylnaphthalenes	45.25	45.82	67.23	39.91	16.20	24.95	13.08	37.63
Trimethylnaphthalenes	50.89	29.70	65.84	64.55	8.82	17.35	6.71	27.22
Alkylated naphthalenes	114.53	90.60	166.32	115.68	29.92	49.27	22.41	77.38
Naphthalene+Alkylated naphthalenes	116.13	91.94	170.58	116.85	30.07	50.54	22.63	77.78
Phenanthrene	11.10	15.69	35.82	14.93	2.12	4.22	0.94	6.79
Methylphenantren	29.02	28.67	64.26	46.09	8.19	11.09	3.89	13.35
Phenanthrene+Methylphenantrenes	40.12	44.36	100.08	61.02	10.31	15.31	4.83	20.14
MPI 1	0.76	0.54	0.52	0.46	1.02	1.10	1.02	0.87
R _C (%)	0.86	0.72	0.71	0.67	1.01	1.06	1.01	0.92
Methylbiphenyls	6.40	8.61	14.45	16.25	1.17	4.66	0.76	4.58
Dimethylbiphenyls	21.17	20.37	31.85	45.18	3.85	13.43	4.23	12.85
Trimethylbiphenyls	17.04	18.90	40.68	55.45	11.35	19.46	13.55	21.54
Alkylated biphenyls	44.61	47.88	86.98	116.88	16.37	37.55	18.54	38.97
Dibenzofuran (DBF)	4.71	5.03	16.03	14.74	1.83	1.92	2.23	3.89
Dibenzothiophene (DBT)	6.77	9.09	17.91	20.34	0.83	1.01	0.94	4.95
Biph / Phen.	0.16	0.19	0.14	0.27	0.11	0.30	0.16	0.23
DBT / PH	0.61	0.58	0.50	1.36	0.39	0.24	0.99	0.73
PAH (+ Alkyl.)	0.00	0.00	0.00	0.00	5.64	7.91	4.49	20.00

^a CPI= (Carbon Preference Index). ^b Pr= Pristane. ^c Ph= Phytane

The main part of the extracts of the investigated coals is composed of asphaltenes (36-68%) - highly reactive components. Quantity of asphaltenes is much higher for coals of low-reduced type. Quantity of asphaltenes decreases during coalification processes and is much higher for coal of low-reduced type. Obviously, their segregation at the early stages of thermal decomposition is very important for the formation of plastic layer and subsequent formation of the coke structure.

Gas chromatography – mass spectrometry analysis of aliphatic and aromatic fractions of the extracts revealed significant quantitative differences in the composition of components extracted from the coking and non-coking coals (Table 5).

Table 5. Composition of extracts obtained from coals under investigation

№	Coal Grade	Type	Coal mine, coal seam	Extract yield (CH ₂ Cl ₂), (µg/g C ₀)	C ₀ , weight (%)	Content of asphaltenes (%)	Content of the aromatic hydrocarbons (%)	Content of the aliphatic hydrocarbons (%)	N+S+O (%)	S ₀ ^{daf} /C ^{daf} (atm)
1	D	LRC	Cheluskintsev, l ₄	10.80	76.7	59	19	5	21	0.0098
2	D	LRC	Trudovskaya, l ₄	10.54	76.3	53	12	4	26	0.0041
3	J	LRC	Gagarina, m ³	1.88	87.8	59	15	13	9	0.0036
4	J	LRC	Zasyad'ko, l ₄	2.08	87.4	68	17	6	14	0.0026
1 ¹	D	RC	Ukraine, k ₈	13.54	71.9	36	24	5	30	0.0105
2 ¹	D	RC	Trudovskaya, k ₈	15.77	69.0	37	15	6	31	0.0260
3 ¹	J	RC	Gagarina, m ₄ ⁰	2.43	87.3	53	30	11	12	0.0071
4 ¹	J	RC	Zasyad'ko, l ₄	2.94	83.6	64	25	6	14	0.0058

The most important task of this work was to divide the influence of rank and the coal-facies on the composition of the extracts, and then to establish their influence on coking ability.

The influence of the coalification degree on the yield and composition of the coal extracts

As it is seen from Table 4 and Fig. 1a, a sharp decrease in the yield of the dichloromethane extract and the content the polar compounds (N + O + S) is observed during the transition from the low-rank to middle-rank coals. We can also see a sharp decrease in the concentration of the following components of hydrocarbons (Table 3):

- *n*-Alkanes (in 6-9 times);
- aromatic compounds, such as naphthalenes, phenanthrenes, biphenyls, and their alkyl-substituted derivatives, especially methyl-substituted (Fig. 1c);
- biomarkers - pristanes, phitanes, steranes, hopanes and diterpenoides.

So, diasteranes and 4 α methylsteranes disappear at the middle stage of metamorphism. The concentration of hopanes, especially $\alpha\beta$ hopanes, decreased to 50 times. Reducing the quantity of 2-3-ringed aromatic compounds in the extract is accompanied by the appearance of polycyclic aromatic compounds (Fig. 1b). This fact shows that highly-condensed aromatic structures are formed during the processes of aromatization at the metamorphism. Some of them go into an insoluble state.

We established the presence of paraffin hydrocarbons with chain length C_{15} - C_{36} for all investigated extracts. The relative distribution of n-alkanes in the extracts is shown in Table. 5. The ratio of components with even and odd number of carbon atoms for chains of different lengths is different, and the carbon preference index (CPI), which characterizes degradation of biological precursors by thermal maturity, varies in the range of 1.15-1.28. It decreases with metamorphism for low-reduced coals and changes a little for the coals of reduced type.

n-Alkanes with shorter chain (C_{15} - C_{19}) dominate in J coals, whereas the long-chain alkanes (C_{27} - C_{31}) dominate in extracts of D-Grade coals. The results are in agreement with existing concepts about the reduction of the proportion of long-chain alkanes during coalification (Matuszewska et. al., 1997).

Influence of coal-facies on the yield and composition of coal extracts

Not only the coals of different metamorphic stages, but isometamorphic samples of different facies (i.e. redox-conditions during deposition) are also distinctly different by the yield dichloromethane extract, which is higher for RC extracts (Fig.1a). These extracts are enriched by aromatic hydrocarbons, heterocompounds, but include lower contents of asphaltenes (Table 4).

The study of the hydrocarbon fractions of RC and LRC extracts showed a significant difference in the quantity of oxygen and sulfur-containing compounds. An absolute content of dibenzothiophenes ($0,94$ - $20,34 \mu\text{g/g } C^{\text{daf}}$) is significantly higher in reduced samples in comparison with low-reduced ($0,83$ - $9,09 \mu\text{g/g } C^{\text{daf}}$) as well as the content of oxygen-containing dibenzofuran (Fig. 2 a,b). In addition, the content of trimethyl-biphenyls is also higher in the extracts of reduced coals (Fig. 2c).

Extracts of coking and non-coking coals differ by the content of steranes and hopanes. Hydrocarbons inheriting the hydrocarbon skeleton of biogenic precursors, are "biological markers", providing information about the sources of organic matter and its transformation processes during coalification (A. Bechtel, W. Puttmann, 1997; Baker, E. W., 1969). The ratios of individual biomarkers at the stage of diagenesis are often used as the indicators of thermal maturity of organic matter (Waples D.W., Machihara T., 1990).

Steranes identified in the studied extracts have 27-29 carbon atoms. Steranes C_{29} are dominating. Their presence indicates the influence of higher terrestrial vegetation (Jauro, N.G., 2007). The concentration of steranes is higher for reduced samples. Especially, a sharp increase of the C_{27} steranes content is observed for reduced coals (in 5-7 times).

Diasteranes are the steranes with skeletal rearrangement of molecules. They were found only in extracts of low-rank coals, first of all in coals of reduced type. The same is true for 4α methylsteranes.

Main geochemical characteristics of investigated coals were calculated based on the above data of GC/MS analysis of coal extracts (Table 4). According to the maturation parameter based on the isomerisation of C_{29} steranes ($20S/(20S+20R)$) an equal rank can be assessed for all low-rank coals. This index is higher for the middle-rank reduced coals, than for low-reduced.

Extracts of J-grade reduced coals differ from LRC extracts by significantly higher content of hopanes, including stereochemically converted, so-called oil-hopanes, with a higher thermodynamic stability ($\alpha\beta$ configuration). The change in the configuration of the aliphatic chain ($22R \rightarrow 22S$) is greater for the samples of reduced type, which is consistent with a high bacterial activity during marine transgressions. The higher steranes/hopanes ratios in this case indicate high primary productivity during sea level rises. These conditions, obviously, favoured the incorporation of O- and S- into aromatic hydrocarbons (as seen from the presence of dibenzofurans and dibenzothiophens).

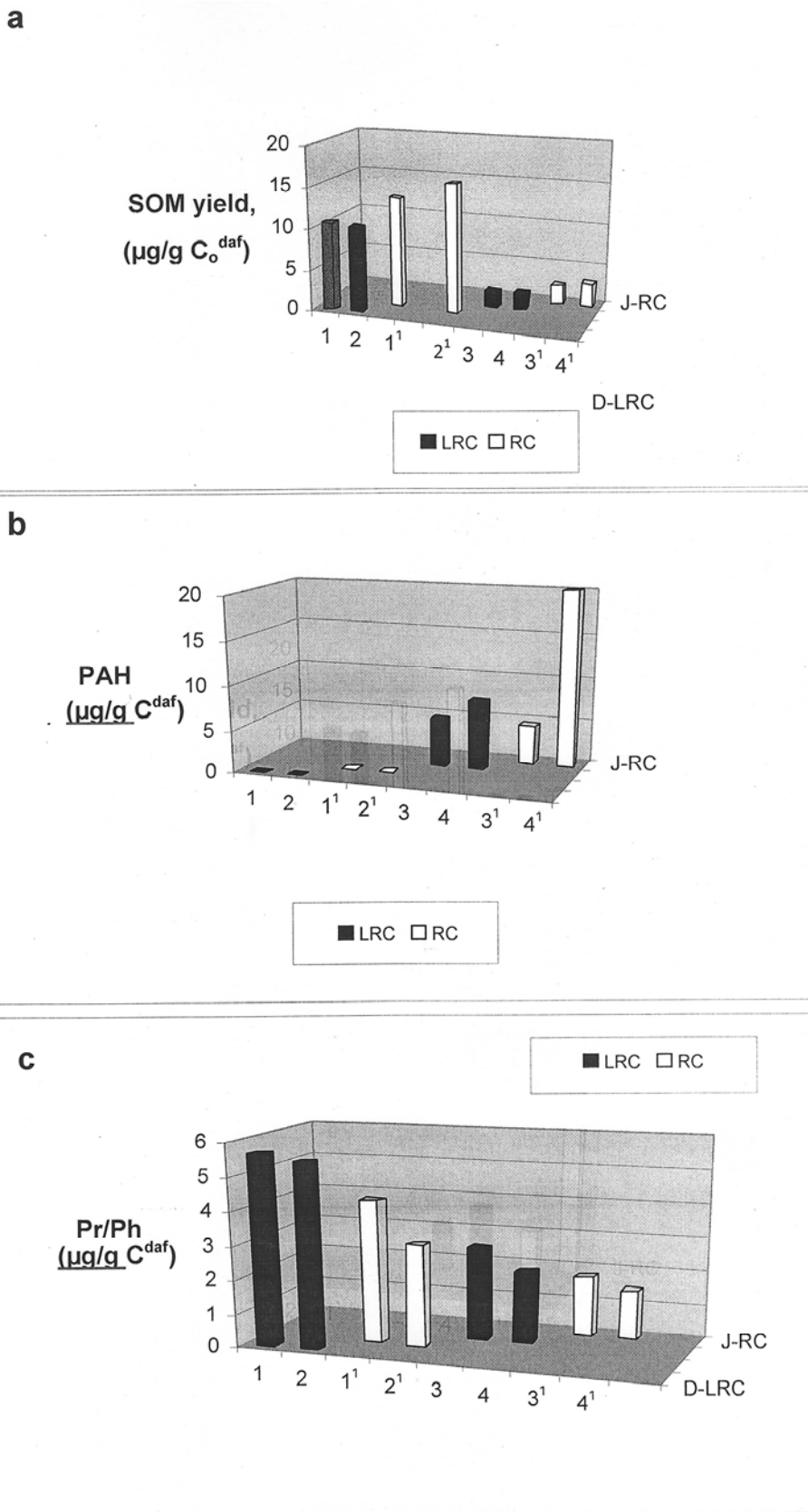
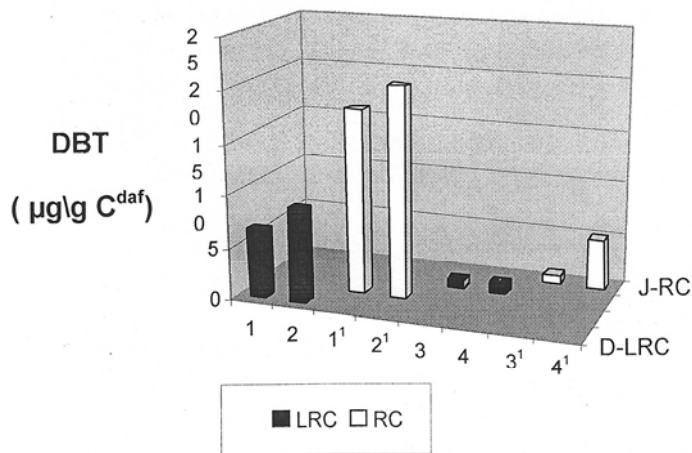
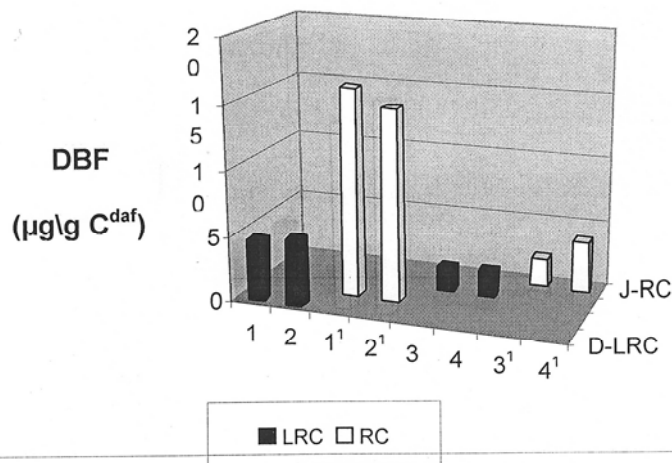


Figure 1 – Content of extractable organic matter (a), PAH (b) and ratio pristane / phytane (c) in extracts of LRC and RC of different coalification degree

a



b



c

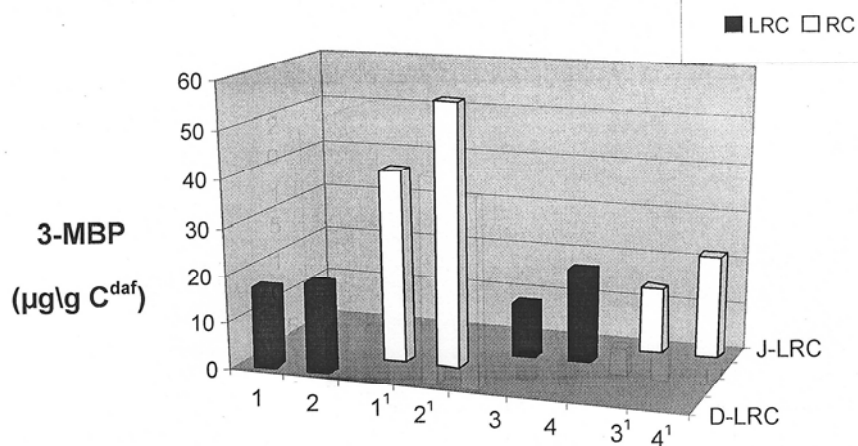


Figure 2 – Main differences in the content of compounds extracted from LRC and RC: a) dibenzothiophene, b) dibenzofuran and c) 3MBP. 3MBP = trimethylbiphenyls

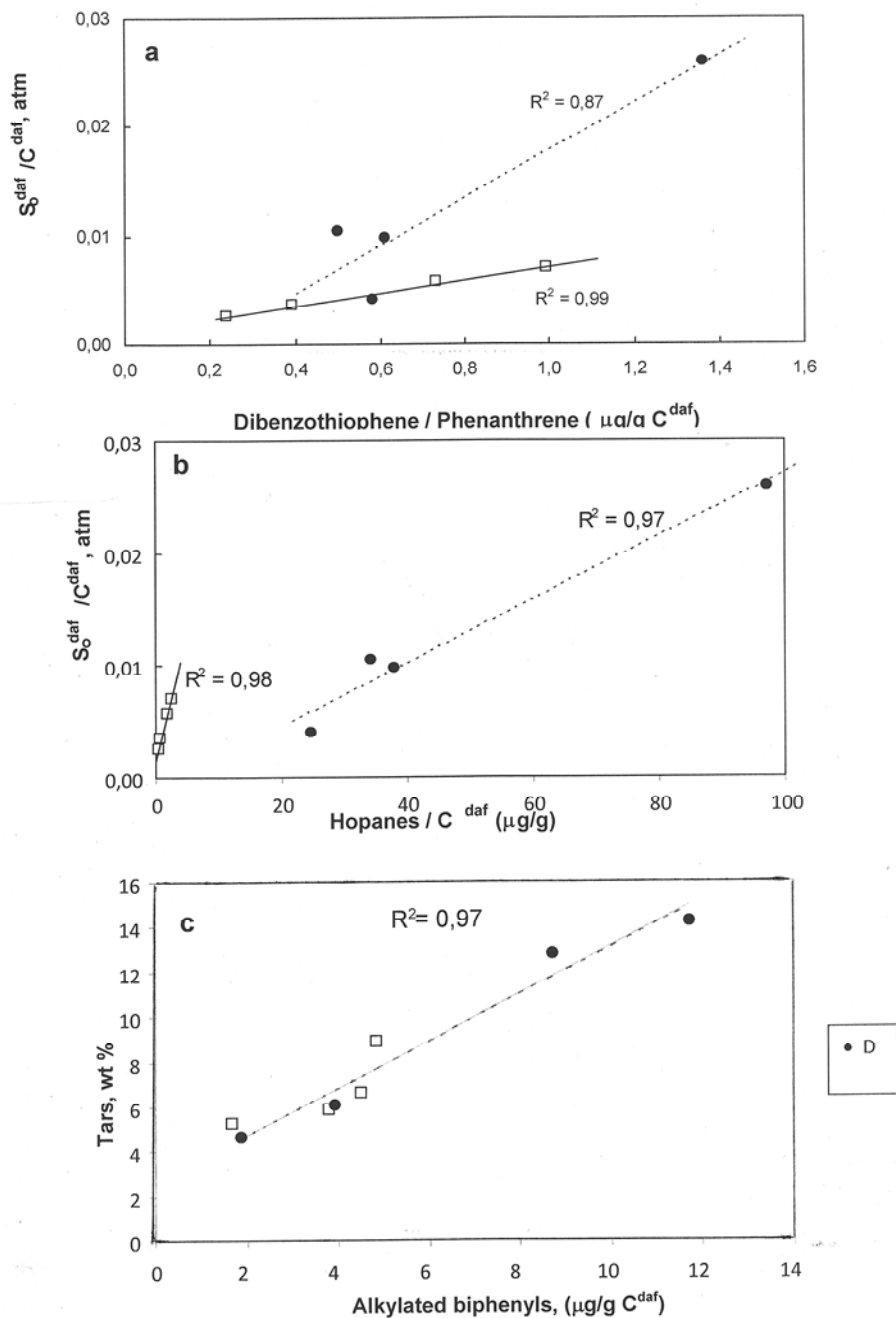


Figure 3 – Geochemical correlations for the studied coals: (a) atomic S_o^{daf}/C^{daf} ratio versus dibenzothiophene / phenanthrene contents, (b) atomic S_o^{daf}/C^{daf} ratio versus hopanenes/organic carbon contents and (c) yield of tars versus alkylated biphenyls. S_o =organic sulphur

Phytane (Ph) and Pristane (Pr) are often regarded as products of reduction or decarboxylation of phytol, a component of chlorophyll, cyanobacteria diphytilovyh esters, some algae and landed shellfish. Typically, the ratio of $Pr/Ph < 1$ is used as a marker of reductive conditions of diagenesis, and $Pr/Ph > 1$ for oxidation conditions (Waples D.W., Machihara T., 1990). The calculated Pr/Ph ratio characterizes a more reducing environment during the organic matter transformation of RC coals.

Influence of coal-facies on the yield and composition of the extracts was evaluated by changes of various characteristics of the extracts, depending on the atomic ratio S_o^{daf}/C^{daf} . A clear

correlation between the declared value and the proportion of sulfur-containing rings in the total quantity of aromatic rings was detected (Fig.3a). This correlation is better for the coals of the middle rank ($R^2=0.99$). In addition, the ratio S_o^{daf}/C^{daf} perfectly correlated with the relative content of hopanes (Fig.3b), so, with high microbial activity during sea transgression. However, the slope of obtained lines is different for coals of different ranks.

Table 6. Yield of semi-coking products, wt %

№	Coal mine, seam	Type	Semi-coke	H ₂ O	Tars	Gas
1	Cheluskintsev, l ₄	LRC	63.5	13.6	6.7	16.2
2	Trudovskaya, l ₄	LRC	64.8	17.5	9.0	8.7
3	Gagarina, m ³	LRC	84.4	2.3	5.3	8
4	Zasyad'ko, l ₄	LRC	82.7	3.2	5.9	8.2
1 ¹	Ukraine, k ₈	RC	62.5	11.3	12.9	13.3
2 ¹	Trudovskaya, k ₈	RC	62.1	10.7	14.3	12.9
3 ¹	Gagarina, m ⁰ ₄	RC	71.8	1	4.7	22.5
4 ¹	Zasyad'ko, k ₈	RC	71.7	1.5	6.1	20.7

Yield of pyrolysis products (Table 6) indicates that a lower content of semi-coke and higher content of tars are formed during semi-coking of the RC in comparison with LRC coals. The amount of gas is practically the same for both types of coals. It is established that the total yield of alkylated biphenyls correlates with the yield of semi coking liquid products (Fig.3c).

Based on the distribution of various classes of compounds in the extracts of coking and non-coking coals, it can be seen that the contents of *n*-alkanes, diterpenoides, naphthalenes, phenantrenes, and polycyclic aromatic hydrocarbons (PAH) allows the characterisation of rank. On the contrary, indicators such as the ratio S_o^{daf}/C^{daf} in coal, the extraction yield, the Pr/Ph ratio, and the contents of hopanes, biphenyls, dibenzofurans and dibenzothiophenes can be used as chemical indicators of coal facies and biogeochemical transformation processes.

Conclusions

1. Obtained results indicate a significant difference in the yield and composition of the extracts for the coking and non-coking coals, caused by differences in redox-conditions during deposition an early diagenesis.
2. Lower Pr/Ph ratios indicate more reductive conditions for reduced coal formation (seawater transgression). These data are consistent with a high content of:
 - hopanes in extracts of RC;
 - dibenzothiophene in extracts of RC;
 - with a lower CPI index in RC in comparison with LRC.
3. More reductive conditions of RC formation are the cause of higher values for the following characteristics:
 - atm. H/C;
 - the quantity of extractable organic matter;
 - concentration of aromatic components in extracts;
4. Appearance of polycyclic aromatic hydrocarbons in the coking coals extracts, increase of the biphenyl, DBT and DBF content for RC may be used for assessment of the technological properties of coals.

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