

## PREDICTING THE YIELD OF COKE AND ITS BYPRODUCTS ON THE BASIS OF ULTIMATE AND PETROGRAPHIC ANALYSIS

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### Abstract

It is established that the yield of coke and its primary byproducts may be predicted on the basis of ultimate and petrographic analysis of the coal (blend) employed. The contribution of individual groups of petrographic components in the coal to the yield of coke and its primary byproducts is determined; coal from the Ukraine, Russia, and the United States is considered. The method developed for predicting the yield of coke and its primary byproducts on the basis of petrographic data is tested at Alchevskkoks and Makeevkoks.

**Keywords:** *coal; ultimate analysis; petrographic analysis; coke yield; byproduct yield.*

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## 1. Introduction

Analysis of the literature on predicting the yield of coke and its primary byproducts permits the following conclusions [1].

- 1) Due to the increased content of petrographically inhomogeneous coal in current coking blend, predicting the yield of coke and its primary byproducts solely on the basis of the volatile matter is no longer satisfactory.
- 2) The yield of coke and its primary byproducts may most expediently be predicted on the basis of ultimate and petrographic analysis of the coal (blend) employed.

## 2. Experimental

In the present work, we consider three samples including coal from Ukraine, Russia, and the United States, which constitutes the bulk of the blend at Ukrainian coke plants [2]. Note that un-oxidized coal is considered, so as to eliminate the influence of oxidation on the yield of coke and its primary byproducts [3–9].

Table 1 presents the maximum, minimum, and mean values of the characteristics for the chosen coal. The mean ash content is greatest for Russian coal ( $A_{me}^d = 8.9\%$ ) and least for Ukrainian coal ( $A_{me}^d = 7.4\%$ ), with a value of 8.5% for coal from the United States. Note that the maximum (41.6–4.2.7%), minimum (16.8–19.3%), and mean (29.8–32.0%) volatile matter is similar for all coals. That indicates similar ranges of this yield in all three groups of coal.

The plastic-layer thickness  $y$  fluctuates broadly for the coal from each country. Table 2 presents the maximum, minimum, and mean values for the content of individual elements and the corresponding structural characteristics [10–18]. We see that the mean content of carbon, hydrogen, and oxygen is similar for the coal samples from Ukraine, Russia, and the United States.

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As expected, the maximum total sulfur content ( $S_{t,me}^d = 1.5\%$ ) and minimum nitrogen content ( $N_{me}^{daf} = 1.6\%$ ) are found for coal from Ukraine, and the minimum total sulfur content ( $S_{t,me}^d = 0.6\%$ ) and maximum nitrogen content ( $N_{me}^{daf} = 2.2\%$ ) for coal from Russia, while the values for coal from the United States are intermediate ( $S_{t,me}^d = 1.0\%$ ;  $N_{me}^{daf} = 1.7\%$ ).

Table 1. Properties of coal samples from Ukraine, Russia, and the United States

Coal source (number of samples)	Value	Proximate analysis, %			Thickness of the plastic layer, mm
		A <sup>d</sup>	S <sup>d</sup> <sub>t</sub>	V <sup>daf</sup>	
Ukraine (40)	Max	13.0	2.99	42.7	29
	Min	2.1	0.48	16.8	6
	Mean	7.4	1.49	32.0	15
Russia (23)	Max	13.3	1.93	41.6	25
	Min	3.9	0.27	19.3	0
	Mean	8.9	0.61	29.8	12
United States (18)	Max	10.0	3.23	42.4	31
	Min	6.8	0.43	17.7	10
	Mean	8.5	0.99	31.6	18
All the coal (81)	Max	13.3	3.23	42.7	31
	Min	2.1	0.27	16.8	0
	Mean	8.1	1.10	31.3	15

Table 2. Ultimate composition and structural parameters of coal samples from Ukraine, Russia, and the United States

Coal source (number of samples)	Value	Ultimate composition, %					Structural parameters	
		C <sup>daf</sup>	H <sup>daf</sup>	N <sup>daf</sup>	S <sup>d</sup> <sub>t</sub>	O <sup>daf</sup> <sub>d</sub>	f <sub>a</sub>	cA
Ukraine (40)	Max	90.3	6.3	2.2	3.0	9.3	0.75	0.81
	Min	81.9	4.1	0.2	0.5	1.3	0.63	0.72
	Mean	86.1	5.6	1.6	1.5	5.2	0.69	0.77
Russia (23)	Max	91,0	6,2	2,8	1,9	9,3	0,75	0,82
	Min	81,7	4,8	1,0	0,3	1,3	0,63	0,72
	Mean	87,3	5,6	2,2	0,6	4,3	0,69	0,78
United States (18)	Max	89,5	6,3	2,3	3,2	5,9	0,74	0,81
	Min	84,2	4,9	1,4	0,4	2,8	0,65	0,74
	Mean	87,0	5,8	1,7	1,0	4,5	0,68	0,77
All the coal (81)	Max	91,0	6,3	2,8	3,2	9,3	0,75	0,81
	Min	81,7	4,1	0,2	0,3	1,3	0,63	0,72
	Mean	86,6	5,7	1,8	1,1	4,8	0,69	0,77

Table 3 presents the maximum, minimum, and mean values of the petrographic characteristics. The coal samples correspond to all metamorphic stages: from  $R_o = 0.58\%$  to  $R_o = 1.77\%$ .

Coal from Ukraine (Table 3) is mainly petrographically uniform ( $Vt_{me} = 84\%$ ), while coal from Russia and the United States is petrographically non-uniform ( $Vt_{me} = 68-69\%$ ). The mean total content of fusinized components is 12%, 30%, and 27% for coal from Ukraine, Russia, and the United States, respectively. The mean liptinite content is low for all the groups ( $L_{me} = 1-4\%$ ), with the exception of some samples from Ukraine ( $L_{me} = 18\%$ ) and the United States ( $L_{me} = 11\%$ ). These characteristics should be reflected in the yield of coke and its primary byproducts from the coal samples.

The yield of coke and its primary byproducts is determined by means of 20-g laboratory apparatus (designed in accordance with the relevant Ukrainian DSTU State Standard [6]). Table 4 presents the experimental values of the yield of coke and its primary byproducts in the dry ash-free state (*daf*). The coke yield in the dry ash-free state (%) is calculated from the formula

$$B_{co}^{daf} = \frac{B_{co}^d - A^d}{100 - A^d} * 100 \quad (1)$$

where  $B_{co}^{daf}$  is the byproduct yield in the dry state, %;  $A^d$  is the ash content of the coal (blend), %. The yield of the byproduct in the dry ash-free state (%) is calculated from the formula

$$B_{bp}^d = \frac{B_{bp}^{daf} * 100}{100 - A^d} \quad (2)$$

where  $B_{bp}^d$  is the byproduct yield in the dry state, %;  $A^d$  is the ash content of the coal (blend), %.

### 3. Results and discussion

According to Table 4, the mean yield of the products is different for the different samples. Thus, for coal from Ukraine, the yield is greatest for hydrogen sulfide and pyrogenetic water; for coal from Russia, the yield is greatest for coke, ammonia, and carbon dioxide; and for coal from the United States, the yield is greatest for tar, raw benzene, nonsaturated hydrocarbons, and gas.

Table 5 shows the pair correlation coefficients for the product yields and the ultimate composition (and also the corresponding structural parameters). For coal from Ukraine, the yield of coke, tar, and raw benzene is determined, to a degree of 71.4–72.7%, by the carbon content (pair correlation coefficients 0.845–0.850); for pyrogenetic water, the correlation is only 65% ( $r = 0.806$ ). The correlation between the product yields and the hydrogen content is weaker: 66.3–70.6%. The correlation of the product yields with the oxygen content is markedly less than for the carbon and hydrogen contents: 37.6–69.89%.

For coal from Russia and the United States, the pair correlation coefficients of the product yields the ultimate composition are higher than for Ukrainian coal; the with determination coefficient is as much as 87.0%.

Note that the structural parameters calculated from the ultimate composition are more closely correlated with the product yields than are the concentrations of individual elements. The yield of coke and its primary byproducts may be most precisely predicted on the basis of the degree  $cA$  of molecular association of the coal. For all the groups of coal, the pair correlation coefficients of  $cA$  are as follow: with the coke yield, 0.889–0.942; with the tar yield – (0.886–0.947); with the raw-benzene yield – (0.894–0.914); and with the yield of pyrogenetic water – (0.833–0.894).

The structural parameters here considered are relatively closely correlated with one another, according to [19]. Any of them may provide a quantitative estimate of the metamorphic stage, aromatic content, and molecular association of the organic mass for a particular coal sample. Hence, to predict the yield of coke and its primary byproducts, we may use a single structural parameter; we might select  $cA$  on account of its particularly close correlation with the yield of coke and its primary byproducts.

Table 6 presents formulas for predicting the yield of coke and its primary byproducts on the basis of  $cA$ , for the groups of coal from Ukraine, Russia, and the United States and for all the samples.

We see that the yield of coke and its primary byproducts may be predicted with sufficient accuracy on the basis of  $cA$ . The formulas for all the coal samples describe the yields as a function of  $cA$  with a multiple-correlation coefficient  $r = 0.855$ – $0.905$  and determination coefficient  $D = 73.1$ – $82.0\%$ . The standard error  $SE$  of the yield calculations is consistent with the requirements of the relevant Ukrainian State Standard.

Table 3. Petrographic characteristics of coal samples from Ukraine, Russia, and the United States

Coal source (number of samples)	Value	Mean vitrinite reflectance $R_{0v}$ , %	Petrographic composition (disregarding mineral impurities), %						Stages of vitrinite metamorphism, %					
			Vt	Sv	I	L	$\Sigma$ FC	<0.50	0.50 -0.64	0.65-0.89	0.90-1.19	1.20-1.39	1.40-1.69	1.70-2.59
Ukraine (4)	Max	1.77	96	1	32	18	32	7	90	98	99	86	96	58
	Min	0.59	53	0	4	0	4	0	0	0	0	0	0	0
	Mean	1.03	84	0	12	4	12	1	12	31	29	14	12	2
Russia (23)	Max	1.60	99	4	83	7	83	11	81	94	91	94	76	18
	Min	0.58	16	0	0	0	0	0	0	0	0	0	0	0
	Mean	1.01	68	1	30	1	30	1	11	23	41	17	6	1
United States (18)	Max	1.56	82	3	40	11	40	1	17	92	95	71	93	4
	Min	0.74	54	0	13	0	0	0	0	0	0	0	0	0
	Mean	1.03	69	1	27	4	27	0	1	26	53	11	8	0
All the coal (81)	Max	1.77	99	4	83	18	83	11	90	98	99	94	96	58
	Min	0.58	16	0	0	0	0	0	0	0	0	0	0	0
	Mean	1.02	76	1	21	3	21	1	9	28	38	14	9	1

Table 4. Yield of coke and its primary byproducts for coal samples from Ukraine, Russia, and the United States

Coal source (number of samples)	Value	Yield of coke and its primary byproducts (daf), %									
		coke	tar	raw benzene	$C_{mH_n}$	$NH_3$	$H_2S$	$CO_2$	$H_2O_{pyr}$	gas	
Ukraine (40)	Max	84.78	7.81	1.83	0.95	0.39	0.92	2.27	5.90	18.09	
	Min	63.79	1.62	0.47	0.33	0.20	0.10	0.19	2.82	8.91	
	Mean	72.34	5.43	1.36	0.63	0.29	0.46	0.88	4.33	14.30	
Russia (23)	Max	81.32	7.80	1.97	1.04	0.73	0.34	3.39	5.71	17.14	
	Min	63.48	1.76	0.44	0.12	0.15	0.03	0.59	1.30	11.48	
	Mean	73.92	4.48	1.17	0.68	0.51	0.13	1.53	3.83	13.76	
United States (18)	Max	83.55	8.23	2.20	1.32	0.46	0.57	1.58	5.17	16.61	
	Min	65.06	2.43	0.43	0.40	0.13	0.03	0.27	1.55	11.07	
	Mean	72.38	5.63	1.43	0.77	0.32	0.25	0.95	3.97	14.31	
All the coal (81)	Max	84.78	8.23	2.20	1.32	0.73	0.92	3.39	5.90	18.09	
	Min	63.48	1.62	0.43	0.12	0.13	0.03	0.19	1.30	5.54	
	Mean	72.80	5.14	1.31	0.70	0.37	0.28	1.12	4.04	14.1	

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Table 5. Pair correlation coefficients

Characteristic	$B_{co}^{daf}$	$B_{tar}^{daf}$	$B_b^{daf}$	$B_{pyr}^{daf}$
Ukraine				
$C^{daf}$	0.848	-0.850	-0.845	-0.806
$H^{daf}$	-0.824	0.814	0.840	0.753
$O^{daf}$	-0.726	0.728	0.720	0.679
$f_a$	0.878	-0.872	-0.885	-0.813
$cA$	0.889	-0.886	-0.894	-0.833
Russia				
$C^{daf}$	0.901	-0.876	-0.892	-0.885
$H^{daf}$	-0.843	0.903	0.790	0.808
$O^{daf}$	-0.836	0.804	0.832	0.811
$f_a$	0.909	-0.930	-0.874	-0.877
$cA$	0.922	-0.929	-0.894	-0.894
United States				
$C^{daf}$	0.935	-0.940	-0.908	-0.811
$H^{daf}$	-0.883	0.889	0.860	0.823
$O^{daf}$	-0.910	0.902	0.893	0.793
$f_a$	0.928	-0.933	-0.905	-0.842
$cA$	0.942	-0.947	-0.914	-0.843
All the coal				
$C^{daf}$	0.861	-0.853	-0.833	-0.843
$H^{daf}$	-0.831	0.850	0.823	0.750
$O^{daf}$	-0.749	0.734	0.795	0.715
$f_a$	0.895	-0.899	-0.873	-0.830
$cA$	0.905	0.906	-0.882	-0.855

Table 6. Formulas for predicting the yield of coke and its primary byproducts on the basis of the structural parameter  $cA$

Source of coal	Formula	Statistical estimates		
		$r$	$D, \%$	$SE, \%$
Ukraine	$B_{co}^{daf} = 216.83cA - 93.489$	0.889	79.1	0.472
	$B_{tar}^{daf} = -64.066cA + 54.427$	0.886	78.4	0.288
	$B_b^{daf} = -12.773cA + 11.124$	0.894	79.9	0.175
	$B_{pyr}^{daf} = -27.226cA + 25.155$	0.833	69.2	0.296
Russia	$B_{co}^{daf} = 192.39cA - 75.262$	0.922	85.0	0.499
	$B_{tar}^{daf} = -63.730cA + 53.903$	0.929	86.3	0.294
	$B_b^{daf} = -14.690cA + 12.559$	0.894	79.9	0.149
	$B_{pyr}^{daf} = -36.900cA + 32.442$	0.894	79.9	0.276
United States	$B_{co}^{daf} = 206.26cA - 86.072$	0.942	88.5	0.469
	$B_{tar}^{daf} = -65.460cA + 55.915$	0.947	89.7	0.274
	$B_b^{daf} = -20.167cA + 16.923$	0.914	83.6	0.134
	$B_{pyr}^{daf} = -31.326cA + 28.034$	0.843	71.0	0.289
All the coal	$B_{co}^{daf} = 204.67cA - 84.501$	0.904	81.8	0.483
	$B_{tar}^{daf} = -65.017cA + 55.176$	0.905	82.0	0.281
	$B_b^{daf} = -14.652cA + 12.581$	0.882	77.8	0.145
	$B_{pyr}^{daf} = -31.808cA + 28.556$	0.855	73.1	0.281

Since the prediction of the yield of coke and its primary byproducts is systematic, while the ultimate composition is not determined in plant laboratories, as a rule, it is expedient to predict the yield of coke and its primary byproducts on the basis of petrographic data, which are routinely gathered in quality control of the coal arriving at the plant [1, 20, 21].

On the basis of experience with petrographic analysis of coal and coking blend, we may establish limits on the vitrinite reflectance corresponding to the ranks of coal generally employed in coking, regardless of the source of the coal. In the analysis of reflectograms, we recommend the table of correspondences proposed in [22].

Note that the composition and structure of inertinite also change with metamorphism of the coal. However, in view of the insignificant changes in its properties on thermal destruction and the instrumental difficulties in determining the stage of development, we only consider the total inertinite content in the coal.

We divide the organic mass into eight groups when determining the contribution of the petrographic components to the yield of coke and its primary byproducts:

- six vitrinite components corresponding to the ranks  $R_o \leq 0.64\%$ ,  $R_o = 0.65\text{--}0.89\%$ ,  $R_o = 0.90\text{--}1.19\%$ ,  $R_o = 1.20\text{--}1.39\%$ ,  $R_o = 1.40\text{--}1.69\%$ , and  $R_o = 1.70\text{--}2.20\%$ ;
- a fusinized component combining inertinite and semivitrinite;
- a liptinite component.

The liptinite corresponding to rank  $R = 1.20\text{--}1.39\%$  is combined with the vitrinite of the same rank, on account of its low content and similar properties [23].

Table 7 presents this division into groups, with the corresponding  $cA$  values, calculated by the solution of the following system of linear equations ( $m$  equations with  $n$  unknowns) on the basis of the Gauss method [24–26]

$$\left\{ \begin{array}{l} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n = b_1, \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n = b_2, \\ \dots\dots\dots \\ a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n = b_m. \end{array} \right. \quad (3)$$

Here the coefficients  $a_{11}, \dots, a_{nm}$  correspond to the content of the specific petrographic groups in the given coal sample, %;  $b_1, \dots, b_m$  are the values of the structural parameter  $cA$  or the yield of coke and its primary byproducts for the given sample;  $x_1, \dots, x_n$  are the values of the structural parameter  $cA$  or the yield of coke and its primary byproducts corresponding to the content of the specific petrographic group.

It appears from Table 7 that, as the vitrinite develops metamorphically, the degree of molecular association of the coal's organic mass increases; the value of  $cA$  is least for liptinite, which is the least structured maceral.

In Table 8 and in the figure 1, we present conversion coefficients from the organic mass of the petrographic components in coal from Ukraine, Russia, and the United States to the organic mass of coke and its primary byproducts; statistical estimates are also provided. Note that the conversion coefficients from the vitrinite component to coke increase from group I to group VI, while the conversion coefficients to tar, raw benzene, and pyrogenetic water decline.

Analysis of the conversion coefficients for groups VII and VIII confirms that the coke yield is lower from liptinite macerals than from inertinite macerals, while the yield of tar, raw benzene, and gas is higher.

On the basis of the combined data for coal from Ukraine, Russia, and the United States, Table 9 presents universal formulas for predicting the yield of coke and its primary byproducts for blend containing coal from different sources; statistical estimates are also provided.

Overall, conversion of the vitrinite component in coal's organic mass to coke, tar, raw benzene, and pyrogenetic water follows familiar patterns: as the coke's level of metamorphic development increases, the coke yield increases, while the yield of tar, raw benzene, and pyrogenetic water declines [27].

Table 7. Division of the coal's organic mass into groups and corresponding mean cA values

Group	Petrographic components in group	Notation and mathematical formula for group	Degree of molecular association cA
I	vitritine $R_0 \leq 0.64\%$	$V_{tI} = (V_t^{< 0.64} V_t) / 100$	0.70
II	vitritine $R_0 = 0.65-0.89\%$	$V_{tII} = (V_t^{0.65-0.89} V_t) / 100$	0.75
III	vitritine $R_0 = 0.90-1.19\%$	$V_{tIII} = (V_t^{0.90-1.19} V_t) / 100$	0.77
IV	vitritine and liptinite $R_0 = 1.20-1.39\%$	$V_{tIV} = (V_t^{1.20-1.39} V_t + L^{1.20-1.39} L) / 100$	0.81
V	vitritine $R_0 = 1.40-1.69\%$	$V_{tV} = (V_t^{1.40-1.69} V_t) / 100$	0.84
VI	vitritine $R_0 = 1.70-2.20\%$	$V_{tVI} = (V_t^{1.70-2.20} V_t) / 100$	0.91
VII	liptinite	$L = (L^{< 0.64} + L^{0.65-0.89} + L^{0.90-1.19}) L / 100$	0.67
VIII	Inertinite and semivitrinite	$I + S_v = I + S_v$	0.78

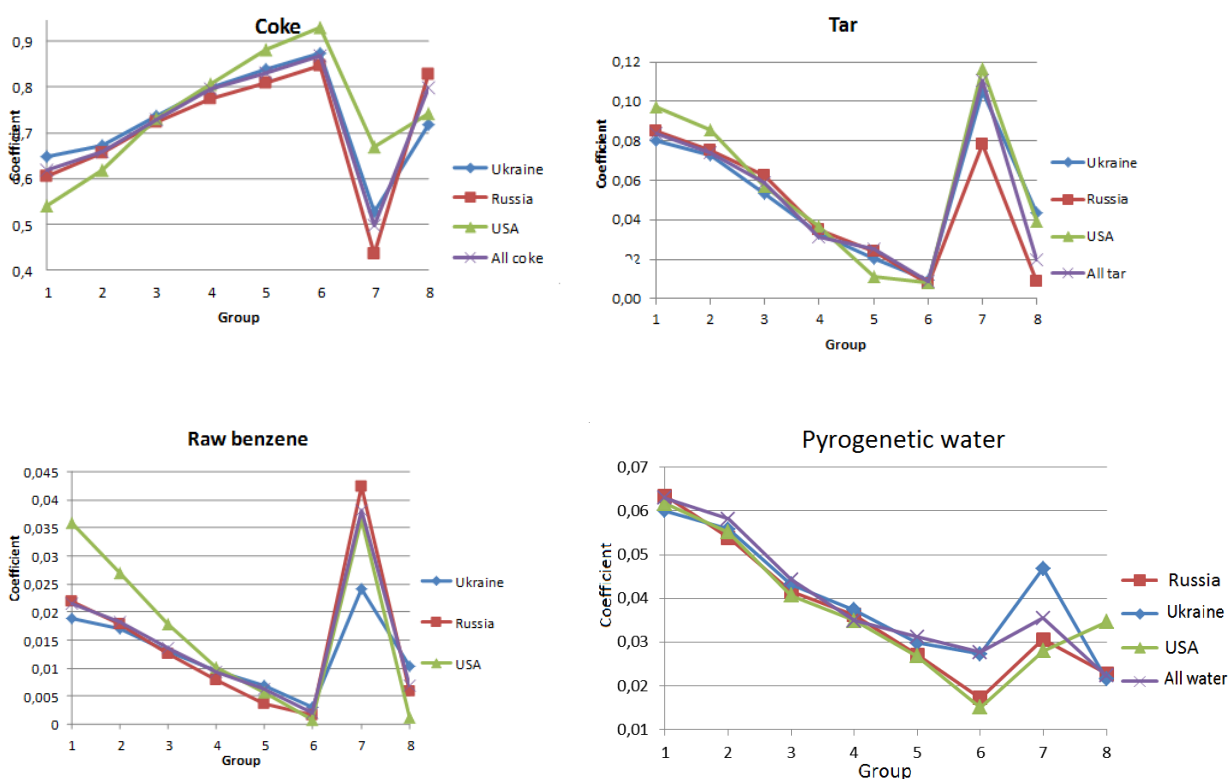


Fig.1. Conversion coefficients from the organic mass of the petrographic components (from Ukraine, Russia and the United States) to the organic mass of coke and its primary byproducts

For the proposed formulas, the correlation coefficients are high (0.970–0.997), as are the determination coefficients (94.0–99.5%). The standard error is 0.41%, 0.28%, 0.09%, and 0.19% in predicting the yield of coke, tar, raw benzene, and pyrogenetic water, respectively. That is within the permissible error according to the relevant Ukrainian State Standard. Hence, the formulas may be regarded as suitable for the prediction of the yield of coke and its primary byproducts on the basis of petrographic analysis.

The proposed prediction method is tested for data from Alchevsk and Makeevsk coke plants. Coke production at Alchevskkoks includes traditional coking of ordinary coal blend (batteries 5–8) with wet slaking of the coke and coking of rammed blend with wet slaking (battery 9) and dry slaking (battery 10) of the coke [28–30]. At Makeevkoks, coking of ordinary coal blend is employed (batteries 1–4), with wet slaking [28, 31–33].

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Table 8. Conversion coefficients from the organic mass of the petrographic components in coals from Ukraine, Russia, and the United States to the organic mass of coke and its primary byproducts

Characteristic	Group								Statistical estimates		
	I	II	III	IV	V	VI	VII	VIII	r	D, %	SE, %
Coal from Ukraine											
B <sup>daf</sup> <sub>co</sub>	0.647 9	0.672 2	0.735 3	0.79793	0.837 9	0.874 1	0.525 7	0.716 5	0.99 8	99. 5	0. 42 8
B <sup>daf</sup> <sub>tar</sub>	0.079 8	0.072 9	0.053 5	0.0333	0.020 4	0.009 4	0.104 8	0.043 6	0.99 6	99. 1	0. 17 0
B <sup>daf</sup> <sub>b</sub>	0.018 8	0.017 0	0.013 0	0.0095	0.006 8	0.003 0	0.024 2	0.010 3	0.97 6	95. 2	0. 08 0
B <sup>daf</sup> <sub>pyr</sub>	0.060 0	0.055 8	0.432	0.0373	0.029 8	0.027 3	0.046 8	0.021 5	0.97 2	94. 5	0. 18 9
Coal from Russia											
B <sup>daf</sup> <sub>co</sub>	0.605 5	0.655 1	0.724 0	0.7736	0.808 7	0.846 7	0.435 7	0.827 5	0.99 9	99. 8	0. 23 7
B <sup>daf</sup> <sub>tar</sub>	0.085 1	0.075 0	0.062 6	0.0352	0.023 9	0.007 3	0.078 0	0.008 9	0.99 6	99. 2	0. 17 5
B <sup>daf</sup> <sub>b</sub>	0.021 9	0.017 9	0.012 5	0.0079	0.003 7	0.001 6	0.042 4	0.005 9	0.98 4	96. 7	0. 08 7
B <sup>daf</sup> <sub>pyr</sub>	0.063 4	0.053 9	0.041 5	0.0362	0.027 1	0.017 2	0.030 6	0.022 8	0.98 7	97. 2	0. 20 0
Coal from United States											
B <sup>daf</sup> <sub>co</sub>	0.539 6	0.618 5	0.730 3	0.8073	0.881 5	0.929 0	0.669 0	0.741 5	0.99 8	99. 7	0. 25 3
B <sup>daf</sup> <sub>tar</sub>	0.097 3	0.085 5	0.056 9	0.0369	0.011 4	0.008 1	0.116 4	0.039 1	0.98 9	97. 7	0. 21 4
B <sup>daf</sup> <sub>b</sub>	0.035 9	0.027 0	0.017 9	0.0101	0.005 7	0.000 7	0.036 6	0.001 2	0.99 2	98. 4	0. 05 8
B <sup>daf</sup> <sub>pyr</sub>	0.061 7	0.055 1	0.040 7	0.0349	0.026 8	0.015 1	0.028 0	0.034 6	0.96 5	93. 1	0. 19 6

Table 9. Formulas for predicting the yield of coke and its primary byproducts on the basis of the petrographic composition of the coals

Formula	Statistical estimates		
	r	D, %	SE, %
$B_{co}^{daf} = 0.6184 V_{tI} + 0.658 V_{tII} + 0.7286 V_{tIII} + 0.7954 V_{tIV} + 0.8298 V_{tV} + 0.8690 V_{tVI} + 0.4978 L + 0.7984 (I + S_v)$	0.997	99.5	0.41
$B_{tar}^{daf} = 0.0838 V_{tI} + 0.0742 V_{tII} + 0.0586 V_{tIII} + 0.0316 V_{tIV} + 0.0254 V_{tV} + 0.0085 V_{tVI} + 0.1105 L + 0.0198 (I + S_v)$	0.987	97.4	0.28
$B_b^{daf} = 0.0215 V_{tI} + 0.0183 V_{tII} + 0.0136 V_{tIII} + 0.0093 V_{tIV} + 0.006 V_{tV} + 0.0019 V_{tVI} + 0.0382 L + 0.0068 (I + S_v)$	0.970	94.0	0.09
$B_{pyr}^{daf} = 0.0630 V_{tI} + 0.0582 V_{tII} + 0.0443 V_{tIII} + 0.0349 V_{tIV} + 0.0312 V_{tV} + 0.0277 V_{tVI} + 0.0355 L + 0.0223 (I + S_v)$	0.973	94.7	0.19



Mean monthly data regarding the proximate analysis of production blend and the yield of coke and its primary byproducts are analyzed. The petrographic characteristics of the mean monthly blend are calculated from its ultimate composition and rank composition, with the utilization of data from coke plants on the petrographic characteristics of coal from individual suppliers employed by the plants.

Table 10 presents the maximum, minimum, and mean values for the technological characteristics of the coal blend supplied to the coke batteries during the test period. We see that, as a result of features of the ramming technology [34-35], the rammed blend sent to batteries 9 and 10 has higher mean working moisture content ( $W_{t,me}^r = 11.3\text{--}11.5\%$ ) than the ordinary blend sent to batteries 5–8 at Alchevskkoks (10.0%) and batteries 1–4 at Makeevkoks (8.7%).

Table 10. Proximate analysis of the coal blends

Battery	Value	Proximate analysis, %				
		$W_t^r$	$A^d$	$S_t^d$	$V^d$	$V^{daf}$
Alchevskkoks						
5-8	Max	11.1	8.8	1.87	30.0	32.8
	Min	8.7	8.1	1.01	24.9	27.2
	Mean	10.0	8.6	1.49	27.4	29.6
9	Max	12.3	8.9	1.54	31.7	34.6
	Min	10.9	7.7	0.92	25.8	28.2
	Mean	11.5	8.4	1.30	28.8	30.7
10	Max	11.5	8.9	1.46	31.7	34.6
	Min	10.9	7.7	0.92	26.3	28.7
	Mean	11.3	8.4	1.27	28.3	30.9
Makeevskoks						
1-4	Max	10.6	8.5	0.91	27.4	29.9
	Min	7.4	7.8	0.70	24.7	26.8
	Mean	8.7	7.9	0.78	25.4	27.6

The ash content and total sulfur content are lower in the rammed blend at Alchevskkoks: 8.4 and 1.27–1.30%, as against 8.6 and 1.49%, respectively, for the ordinary blend. On account of the elevated content of high volatile coal in the rammed blend, the volatile matter (in the dry ash-free state) is higher: 30.7–30.9%, on average, as against 29.6% and 27.6% for the ordinary blend (Table 10).

Table 11 presents the petrographic characteristics of the coal blend used in statistical analysis. The blend in batteries 5–8 is characterized by a mean vitrinite reflectance of 1.05%. The blend contains 79% vitrinite-group macerals and 19% fisinised components.

The coal blend at batteries 9 and 10 is characterized by low vitrinite reflectance (0.97%). Ramming permits the use of a high proportion of petrographically inhomogeneous coal in the blend, as is evident from the content of fisinised components ( $\Sigma FC_{me} = 25\%$ ). The elevated content of vitrinite corresponding high volatile coals (51%) should lead to decrease in coke yield and increase in the yield of its primary byproducts in comparison with the blend at batteries 5–8.

The mean vitrinite reflectance of the blend at Makeevkoks is 1.11%. The blend contains 85% vitrinite-group macerals and 13% lean components.

Table 12 presents the production information regarding the yield of coke and its primary byproducts that is subjected to statistical analysis. The yield data are presented for the dry ( $d$ ) and dry ash-free ( $daf$ ) states.

Conversion of data from the dry state to the ash-free state eliminates the influence of the ash content in the blend on the yield of coke and its primary byproducts and hence the chemical potential of solely the coal's organic component may be assessed, as shown in [6].

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Table 11. Petrographic characteristics of coal blends

Battery	Value	Mean vitrinite reflectance $R_0$ , %	Petrographic composition, %			Stages of vitrinite metamorphism, %								
			$V_t$	$S_v$	I	L	$\Sigma FC$	<0.50	0.50-0.64	0.65-0.89	0.90-1.19	1.20-1.39	1.40-1.69	1.70-2.59
Alchevskkoks														
5-8	Max	1.17	86	2	23	3	24	1	7	40	57	39	25	2
	Min	0.96	73	0	11	1	12	0	2	19	17	6	1	0
	Mean	1.05	79	1	18	2	19	0	4	28	41	17	9	1
9	Max	1.13	82	1	31	6	32	2	14	53	46	10	28	6
	Min	0.89	65	0	15	2	15	0	4	31	24	2	0	0
	Mean	0.97	71	1	25	3	25	1	9	41	35	7	6	2
10	Max	1.13	82	1	31	6	32	2	14	53	46	10	28	6
	Min	0.89	65	0	15	2	15	0	4	31	24	2	0	0
	Mean	0.97	71	1	25	3	25	1	9	41	35	7	6	2
Makeevskkoks														
1-4	Max	1.18	89	1	17	2	18	2	16	6	91	34	3	0
	Min	0.97	80	0	9	1	10	0	0	0	60	7	0	0
	Mean	1.11	85	0	13	2	13	0	3	3	75	19	0	0

Table 12. Yield of coke and its primary byproducts for coal samples

Battery	Value	Yield of coke and its primary byproducts, %						
		$B_{co}^d$	$B_{daf_{co}}^d$	$B_{daf_{tar}}^d$	$B_{tar}^d$	$B_{daf_{tar}}^d$	$B_{daf_b}^d$	$B_{daf_b}^d$
Alchevskkoks								
5-8	Max	78.49	76.59	4.48	4.89	1.30	1.42	1.42
	Min	76.05	73.83	9.92	3.20	0.98	1.07	1.07
	Mean	77.24	75.11	3.61	3.95	1.13	1.23	1.23
9	Max	76.06	73.78	4.75	5.18	1.39	1.52	1.52
	Min	72.71	70.21	3.09	3.39	1.04	1.13	1.13
	Mean	74.22	71.87	3.82	4.17	1.19	1.30	1.30
10	Max	74.66	72.25	4.75	5.18	1.39	1.52	1.52
	Min	71.62	68.99	3.09	3.39	1.04	1.13	1.13
	Mean	72.71	70.23	3.82	4.17	1.19	1.30	1.30
Makeevskkoks								
1-4	Max	80.39	78.72	3.79	4.13	1.28	1.39	1.39
	Min	75.98	73.83	3.11	3.38	1.04	1.13	1.13
	Mean	77.68	75.75	3.41	3.70	1.15	1.25	1.25

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The mean coke yield, in both the dry state and the dry ash-free state, is higher for ordinary blend than for rammed blend. Dry slaking at coke battery 10 reduces the coke yield by 1.42% (in the dry state) and 1.64% (in the dry ash-free state) in comparison with battery 9. Note that, on account of the large volatile matter from the blend in batteries 9 and 10, the yield of tar and raw benzene is also higher than for batteries 5–8 at Alchevskkoks and 1–4 at Makeevkoks.

To compare the laboratory and plant yields of coke and its primary byproducts, the petrographic characteristics calculated for the mean monthly production blend at Alchevskkoks and Makeevkoks are substituted into the formulas in Table 9.

The calculation results are compared with plant data regarding the yields, and the mean conversion coefficients from laboratory values to production data are calculated. Thus, for conversion from the calculated yields of coke and its primary byproducts to production data, we use the coefficients

$$k_i = B^{pr}_i / B^{ca}_i, \quad (4)$$

where  $B^{pr}_i$  is the production value of the yield of coke and its primary byproducts, %;  $B^{ca}_i$  is the calculated value of the yield of coke and its primary byproducts, %.

The mean conversion coefficient from the calculated total yield of coke and its primary byproducts to the production value is

$$\bar{k} = \frac{k_1 + \dots + k_i}{i} \quad (5)$$

where  $i$  is the number of values used in the calculations.

Table 13 presents the mean error in calculating the yield of coke and its primary byproducts. We see in Table 13 that the yield of coke obtained in laboratory conditions is close to the production value ( $k = 0.9763$ – $1.0200$ ). The yield of tar and raw benzene in laboratory conditions is overestimated:  $k = 0.7851$ – $0.7914$  and  $0.9423$ – $0.9618$ , respectively. That confirms the following opinion [36]: “The laboratory yields cannot agree precisely with the production values since loss of chemical products is inevitable in plant conditions but is minimized in laboratory conditions.”

Table 13. Conversion coefficients from laboratory (calculated) values to plant values

Battery	Product	Conversion coefficient	Standard error SE, %
Alchevskkoks			
5-8	$B^{daf}_{co}$	1.0227	0.384
	$B^{daf}_{tar}$	0.7914	0.134
	$B^{daf}_b$	0.9618	0.049
9	$B^{daf}_{co}$	0.9991	0.290
	$B^{daf}_{tar}$	0.7851	0.111
	$B^{daf}_b$	0.9423	0.036
10	$B^{daf}_{co}$	0.9763	0.290
	$B^{daf}_{tar}$	0.7851	0.111
	$B^{daf}_b$	0.9423	0.036
Makeevskoks			
1-4	$B^{daf}_{co}$	1.0230	0.408
	$B^{daf}_{tar}$	0.7326	0.168
	$B^{daf}_b$	0.9945	0.041

Analysis of the production yields of coke, tar, and raw benzene and laboratory yields (for a five-section furnace, in accordance with State Standard GOST 18635–73 [37]) from blend of the same quality indicates that the coke yield in laboratory conditions agrees with the production yields at a level of 99%, with figures of 89% and 96% for tar and raw benzene [36].

Thus, the relations between the laboratory and production values obtained in the present work and in [36] are very close [38].

On the basis of the research at Alchevskkoks and Makeevkoks, methods of calculating the yield of coke and its primary byproducts on the basis of petrographic analysis of the blend have been developed, with allowance for the conditions of blend preparation and coke slaking.

#### 4. Conclusions

- (1) We have established theoretically and confirmed experimentally that the yield of coke and its primary byproducts may be predicted on the basis of ultimate and petrographic analysis of the coal (blend) employed.
- (2) We have determined the contribution of individual groups of petrographic components in coal from the Ukraine, Russia, and the United States to the yield of coke and its primary byproducts.
- (3) The method developed for predicting the yield of coke and its primary byproducts on the basis of petrographic data has been tested at Alchevskkoks and Makeevkoks.

#### Symbols

$A^d$	ash content of coal in the dry state, %;
$V^{daf}$	volatile matter in the dry ash-free state, %;
$S_t^d$	sulphur of coal in the dry state, %;
$cA$	the degree of molecular association;
$f_a$	the aromatic content of the structure;
$R_0$	mean vitrinite reflection coefficient, %;
$Vt$	vitrinite, %;
$Sv$	semivitrinite, %;
$I$	inertinite, %;
$L$	liptinite, %;
$\Sigma FC$	sum of fusinized components, %;
$y$	thickness of the plastic layer, mm;
$r$	multicorrelation coefficient;
$D$	determination coefficient, %;
$SE$	standard error, %.
$B_{cor}^{daf}, B_{tar}^{daf}, B_{br}^{daf}, B_{pyrr}^{daf}$	the yield of coke, tar, raw benzene and pyrogenetic water, %;
$C^{daf}, H^{daf}, N^{daf}, O^{daf}_d$	carbon, hydrogen, nitrogen and oxygen in the dry, ash-free state, %;

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