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THE UNIFIED METHOD OF CALCULATION THE THERMODINAMIC FUNCTIONS OF THE INTERMEDIATE FRACTION OF COAL TAR

Abstract. Separate isolated organic compounds with a known molecular structure as well as a unified additive method (UAM) have been used in order to calculate the thermodynamic functions of heat capacity$C_p(T)$, of enthalpy $\Delta H(T)$and entropy S(T) and of Gibbs free energy $\Delta G_f(T)$ for heavy raw materials. The datawere used thatachieved using elemental analysis and quantitative analysis of chromatography-mass spectrometryfor determining the thermodynamic functions of the process ofcoal tar cavitation of by UAM. The nature of the unified additive method is to consider the unit mass of a molecule or a complex molecular systems as the unit mass of individual structural fragments transferred from one system to another. Comparison of the results of calculations of thermodynamic functions obtained by UAM with reference data showed that they are well compatible, which, in turn, gives grounds for applying the unified additive method to complex systems.

Keywords: unified additive method, thermodynamic functions, coal tar, cavitation, hydroconversion reaction.

The thermodynamic properties of complex organic systems are an important parameter in modeling their processing. For this, it is necessary to develop simple methods for calculating thermodynamic functions. This is especially important for processing of complex raw materials.

The additive method for calculating the thermodynamic functions of organic molecules, proposed in this work [1-3], was adapted and prepared for its application to heavy raw materials of complex composition. The proposed method is based on an additive scheme, where the set of parameters is determined from the hybrid states of carbon atoms and the number of chemically bonded hydrogen atoms when calculating the temperature dependence of the thermodynamic functions of free-form hydrocarbons at temperatures from 298 to 1000 K[4].

The aim of the work is to determine the thermodynamic functions of the average fractionof coal tar cavitation processing by using a unified additive method.

EXPERIMENTAL PART

In order to study the thermodynamic properties of the average fraction cavitation process at 230-300°C from high-temperature coal tar, the component composition of the fraction was analyzed using the method of chromatography-mass spectrometry (CMS). The number of structural fragments in the fractional composition of coal tar was determined using data obtained by CMS analysis. The composition of the coal tar intermediate fraction at 230-300 °Cis presented in work [5].

It is known that thermodynamic functions possess the additive properties of heat capacity C_p, enthalpy ΔH, entropy S, Gibbs free energy ΔG, reduced Gibbs free energy $(G\text{-}H_{298})/T$ and their values are equal to the sum of the thermodynamic functions of any individual elements[6-8].

In this case, any additive property $\Psi$of the substance can be expressed as a linearly dependent function $\xi_i$to its components:

$$\Psi_j = \sum_i^n x_i \xi_i \, ; j = 1,2, \dots \dots, m \; and \; i = 1,2, \dots ., n \qquad (1)$$

wherex_i is the number of the its structural fragment in the test molecule j, and ξ_i is its contribution to the property, m is the number of test molecules selected to find the value of the i- structural fragment.

The temperature dependence of the specific heat ξ_i for a structural fragment is given by the following equation:

$$C_p(\xi_i) = a_i + b_i T + c_i T^2$$

The heat capacity, entropy, enthalpy, and Gibbs free energy are calculated for molecule M using function (1) at temperature T:

$$\Delta C_{p,M}(T) = C_{p,M}(T) - \sum_A C_{p,A}(T)$$

$$\Delta S_M(T) = S_M(T) - \sum_A S_A(T)$$

$$\Delta H_M(T) = \Delta H_{f,298} + \int_{298}^{T_2} \Delta C_{p,M}(T)$$

$$\Delta S_M(T) = \Delta S_{298} + \int_{298}^{T_2} \Delta C_{p,M}(T) d(ln\, T)$$

$$\Delta G(T) = \Delta H(T) - T\Delta S(T)$$

The hydrocarbon portion of organic compounds is formed by structural fragments, and heteroatoms are considered in fragments:

By selecting the structural fragments of a complex organic compound, it is possible to construct the structure of the compounds in a complex organic system and obtain the results of calculations of the thermodynamic functions of the molecules [9-12].

A unified additive method (UAM) is used to calculate the thermodynamic functions of molecules consisting of a set of defined fragments and processes occurring in a complex system consisting of these molecules.

RESULTS AND DISCUSSION

At the first stage of the study, the calculationresults of thermodynamic functions were compared with literature data on the example of a model molecule of 1-methylnaphthalene, which is a component of the intermediate fraction of coal tar

to determine the thermodynamic parameters (table 1). For the calculation, the empirical formula was used for the number of atoms and structural fragments of 1-methylnaphthalene:

Table 1 – Comparison of the thermodynamic functions of a 1-methylnaphthalene molecule with reference data

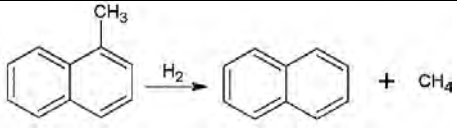
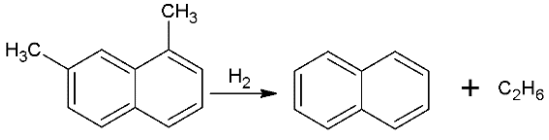
T, K	C_p, kal/mol K		S, kal/mol K		ΔH_f, kcal/mol		ΔG_f, kcal/mol	
	UAM	based on[13]	UAM	based on[13]	UAM	based on[13]	UAM	based on[13]
298	37.77	38.13	95.84	90.21	27.49	27.93	50.05	52.03
300	38.03	38.37	96.09	90.45	27.45	27.89	50.19	52.17
400	49.48	50.74	108.63	103.23	25.65	26.13	57.69	60.54
500	59.57	61.25	120.78	115.72	24.15	24.8	65.91	69.30
600	68.29	69.79	132.43	127.66	22.93	23.71	74.60	78.20
700	75.65	76.76	143.53	138.96	21.97	22.88	83.55	87.47
800	81.63	82.48	154.04	149.59	21.23	22.26	92.51	96.73
900	86.24	87.19	163.93	159.59	20.7	21.83	101.29	106.07
1000	89.47	91.21	173.2	168.99	20.34	21.61	109.64	115.46

According to table 1, the reference data show that satisfactory results of temperature dependence of thermodynamic functions can be achieved with UAM.Therefore, the values of the enthalpy $DH_{r,400}$ of the dealkylation reactions occurring during the cavitation of the intermediate fraction of coal tar with the aid of UAM were determined by the formula (2) below [14,15].

$$\Delta \mathrm{H}^0_{r,400} = \Delta \mathrm{H}^0_{r,298} + (\sum_{prod.}(\mathrm{H}^0_{f,400} - \mathrm{H}^0_{f,298}) - \sum_{init.}(\mathrm{H}^0_{f,400} - \mathrm{H}^0_{f,298})) \quad (2)$$

Table 2 compares the enthalpy valuesat DH_{400} with the control data of the dealkylation reactions that occur during cavitation of the intermediate fraction ofcoal tar determined by the UAM. As can be seen, the results of the UAM calculations are corresponded well with the reference data.

Table 2 – Comparative analysis of the enthalpy DH_{400} of dealkylation reactions occurring during cavitation of the coal tar intermediate fraction by the UAM

№	The reaction	Based on [13]	UAM
		kcal/mol	
1		-9.55	-9.76
2		-3.69	-3.63

The thermodynamic probability of dealkylation reactions that occurs as a result of cavitation processing in the temperature range of T = 400 K, is also analyzed in table 2. The Gibbs energy $\Delta G_p$of (1-2)reactions was calculated from the data given in table 3.

Table 3 – Temperature dependence of Gibbs energy ΔG_p for reaction components 1-2

T, K	ΔG_p, kcal/mol				
	1-methylnaphthalene	1,7-dimethylnaphthalene	naphthalene	methane	ethane
298	52.03	51.08	53.44	-12.15	-7.87
300	52.17	51.27	53.55	-12.11	-7.79
400	60.54	62.18	59.62	-10.07	-3.45
500	69.30	73.53	66.04	-7.85	1.16
600	78.20	85.17	72.66	-5.51	5.96
700	87.47	97.02	79.45	-3.06	10.90
800	96.73	108.96	86.32	-0.56	15.91
900	106.07	121.00	93.26	1.99	21.00
1000	115.46	133.08	100.25	4.58	26.13

As can be seen from figure 1, the probability of thermodynamic reactions 1 and 2 (dealkylation reactions) in the temperature zone T = 400 K is high.

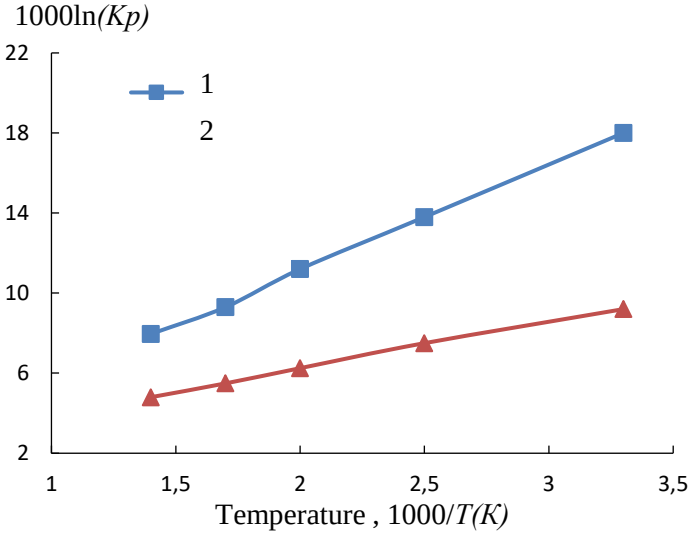


Figure 1 – The dependence of the logarithm of the equilibrium constant ln(K_p) of reactions 1–2 on the temperature 1/T (the reaction number corresponds to table 1)

As mentioned above, the UAMis used to calculate the thermodynamic functions of complex systems, such as heavy raw materials. Assuming that the empirical formula of complex organic compounds consisting of atoms of elements C, H, N, O, S, where *x* = C(%)/12, *y* = H(%), *m* = N(%)/14, *n* = O(%)/16 and*z* = S(%)/32, is

expressed as $C_xH_yN_mO_nS_z$, respectively, the molecular mass M of this complex system is calculated by atomic masses:

$$12n_C + n_H + 14n_N + 16n_O + 32n_S = M \quad (3)$$

where $n_C = x;\ n_H = y;\ n_N = m;\ n_O = n;\ n_S = z$.

The structural characteristics of the compounds for heavy raw materials are studied for a given mass (for example, 100 g). Accordingto the empirical formula based on elemental analysis, the formula can be written as follows:

$$12n_C + n_H + 14n_N + 16n_O + 32n_S = 100 \quad (4)$$

The number of specified structural fragments in the products of the the coal fraction hydroconversion was determined on the basis of quantitative analysis by chromatography-mass spectrometry. The procedure for determining the number of structural fragments per unit mass of heavy raw materials can be simplified using the results of the analysis of CMS, shown in table 1.

The number of atoms and the number of structural fragments in the intermediate fraction of 1 kg of coal tar, calculated according to the CMS analysis, are shown in table 4.

Table 4 – The results of calculating the number of atoms and the number of structural fragments in the intermediate fraction per 1 kg coal tar

Structural parameters	Value	Structural parameters	Value
C	11.654	N	0.105
H	9.68	-NH-	0.105
$H_2C<$	0.468	>C=	3.31
H_3C-	0.38	-HC=	7.493

According to table 4, the empirical formula for the intermediate fraction of 1 kg coal tar is expressed with$C_{11.654}H_{9.68}N_{0.105}$.

There should be noted that within the limits of the accepted structural fragments, it is impossible to isolate the isomers and condensation forms “intermediate statistical structural units”. However, it can be said that the thermodynamic functions of all isomers of the same structure corresponding to the structural fragments that shown in table 4 have close values. This is clear from table 5, where $\Delta H_{f,298}$ values are given for cases where two methyl groups are present in different carbon atoms in the example of dimethylnaphthalene (DMN). From the point of view of structural fragments, these isomers have the same formula, accordingly, the additive method cannot distinguish between them: $\Delta H_{f,298}$ = 18.9 kcal/mol.

Table 5 – The ΔH_{298} values of dimethylnaphthalene isomers in the presence of methyl groups at different carbon atoms [13]

Isomer	$\Delta H_{f,298}$, kcal/mol		Isomer	$\Delta H_{f,298}$, kcal/mol
1,5-DMN	19.55		2,3-DMN	19.97
1,6-DMN	19.72		2,6-DMN	19.72
1,7-DMN	19.55		2,7-DMN	19.72

The values of the thermodynamic functions of the intermediate fraction of coal tar, calculated on the basis of the elemental composition and structural fragments, are shown in table 6.

Table 6 – Molecular Weight M = 151 thermodynamic functions of the intermediate fraction of coal tar

T, K	C_p, cal/mol K	*S*, cal/mol K	ΔH_f, kcal/mol	ΔG_f, kcal/mol
298	39.449	36.253	89.558	60.166
300	39.704	36.215	89.823	60.317
400	51.741	34.519	102.929	68.275
500	62.299	33.137	115.636	76.906
600	71.377	32.040	127.819	85.981
700	78.976	31.196	139.412	95.281
800	85.095	30.575	150.374	104.594
900	89.735	30.146	160.679	113.709
1000	92.896	29.879	170.310	122.417

Conclusions. In conclusion, UAM was used to calculate thermodynamic functions for isolated organic compounds with a known molecular structure, as well as for heavy raw materials.The datawere used that achieved using elemental analysis and quantitative analysis of chromatography-mass spectrometry for determining the thermodynamic functions of the process of coal tar cavitation of by UAM. As a result, the number of structural fragments in the coal tar fraction was determined from the data obtained. The thermodynamic functions of the intermediate fraction of coal tar at a temperature of 230-300°C are determined on the basis of the elemental composition and structural fragments. It was found that the enthalpy values of DH_{400} of the dealkylation reactions occurring at T = 400K during the cavitation of the intermediate fraction of coal tar determined by the UAM method are corresponded well with the reference data. The researches have also shown that unified additive methods based on the calculation of thermodynamic functions are also effective in modelling the direction and probabilities of typical reactions in the processing of heavy raw materials.

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Резюме

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ТАСКӨМІР ШАЙЫРЫ ОРТА ФРАКЦИЯСЫНЫҢ ТЕРМОДИНАМИКАЛЫҚ ФУНКЦИЯЛАРЫН ЕСЕПТЕУДІҢ УНИФИЦИРЛЕНГЕН ӘДІСІ

Белгілі молекулалық құрылымы бар жеке оқшауланған органикалық қосылыстар, сондай-ақ ауыр шикізат үшін де термодинамикалық функцияларды $C_p(T)$ жылу сыйымдылығын, $\Delta H(T)$ энтальпия, $S(T)$ энтропия және еркін $\Delta G(T)$ Гиббс энергиясын есептеудің унифицирленген аддитивті әдісі (УАӘ) әзірленді. УАӘ арқылы таскөмір шайырын кавитациялық өңдеу процесінің термодинамикалық функцияларын анықтауда элементтік анализ және хромато-масс-спектроскопия сандық анализ әдісінің көмегімен анықталған мәліметтер пайдаланылды. УАӘ мәні молекула немесе күрделі құрылымды молекулалар қоспасы массасының бірлігін бір жүйеден екіншісіне ауыстырылатын жеке құрылымдық фрагменттер массасының бірлігі

ретінде қарастыру болып табылады. УАӘ арқылы алынған термодинамикалық функцияларды есептеу нәтижелерін анықтамалық деректермен салыстыру олардың жақсы үйлесетінін көрсетті, бұл, сәйкесінше, УАӘ-ті күрделі жүйелерге қолдануға негіз береді.

Түйін сөздер: унифицирленген аддитивті әдіс, термодинамикалық функциялар, таскөмір шайыры, кавитация, гидроконверсия реакциясы.

Резюме

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УНИФИЦИРОВАННЫЙ МЕТОД РАСЧЕТА ТЕРМОДИНАМИЧЕСКИХ ФУНКЦИЙ СРЕДНЕЙ ФРАКЦИИ КАМЕННОУГОЛЬНОЙ СМОЛЫ

Для расчета термодинамических функций теплоемкости $C_p(T)$, энтальпии $\Delta H(T)$, энтропии $S(T)$и свободной энергии Гиббса $\Delta G(T)$ как отдельных изолированных органических соединений с известной молекулярной структурой, так и тяжелого сырья был использован унифицированный аддитивный метод (УАМ). Для определения термодинамических функций процесса кавитационной обработки средней фракции каменноугольной смолы методом УАМ были использованы данные, полученные с помощью элементного анализа и количественного анализа хромато-масс-спектрометрии. Суть УАМ заключается в том, что молекула или единица массы смеси молекул со сложной структурой представляется как единица массы отдельных структурных фрагментов, которые переносятся из одной системы в другую. Сопоставление результатов расчетов термодинамических функций, полученных с помощью УАМ, со справочными данными показало, что они хорошо совместимы, что, в свою очередь, дает основание применять УАМ к сложным системам.

Ключевые слова: унифицированный аддитивный метод, термодинамические функции, каменноугольная смола, кавитация, реакции гидроконверсии.