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Structural, Physical, and Chemical Properties of Acetylene Production Secondary Raw Materials (Ace) and Their Application in Composite Elastomers

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Abstract:

The objective of this study is to comprehensively investigate the structural, physicochemical, and functional properties of secondary raw materials obtained from acetylene production (VSPA) and to assess their suitability and effectiveness as active carbon fillers in composite elastomeric materials. Special attention is given to the relationship between surface chemistry, morphology, and reinforcing ability in elastomer systems.

The subject of research was VSPA obtained during the pyrolysis of natural gas. A variety of instrumental and analytical techniques were used to gain an in-depth understanding of the material. Chemical composition was examined by elemental analysis, the surface functional groups and aromatic structural were observed by FTIR as well as PMR spectroscopy and the paramagnetic properties of the particle were investigated using EPR technique. Nitrogen, phenol, and CTAB adsorption methods were used to measure the specific surface area and adsorption capacity. Morphology features such as particle size distribution, average particle diameter, bulk density and dispersity were also investigated. Furthermore, the toluene-soluble low-molecular hyper static oligomers were extracted and analyzed for their chemical structure and reactivity. The materials were compared systematically with ones of industrial technical carbon types (T 900, P 701, P 705 and P 803).

Results show that VSPA has good degree of particle dispersion, high specific surface area and higher content of oxygen and hydrogen functional groups. The extracted oligomer (12–15 wt. %, $M \leq 1000$) with carboxyl, phenolic, quinone and lactone groups that can strongly interact with the polymer matrix. The high iodine numbers and oil absorption values are believed to bear witness of rougher surfaces and higher polyconjugation, which will favor the spreadability and adhesion within elastomeric systems.

A new theoretical approach and model VSPA particle, based on microencapsulated core shel structure with a carbon-based core and polymer–oligomer shell system are presented in this study, thus increasing the computational insight on functionalized carbon fillers.

VSPA is an encouraging as well as cost-efficient and sustainable substitute for traditional carbon fillers, with the potential to promote waste valorization and environmentally friendly material design in rubber processing.

The study is confined to laboratory scale tests and further research will be required for an evaluation of the processing characteristics and long-term performance of VSPA filled elastomers under industrial/service conditions.

Keywords: VSPA, acetylene production waste, carbon fillers, elastomer composites, surface functional groups.

Introduction

Carbon fillers are the most important constituents used in the production of composite elastomer materials, determining to a large extent both tecnological aspects (and final working describe herein mechanics and physical) and exploitation characteristics of rubber goods. Technical carbon (carbon black) with different particle size was commonly employed in the rubber industry for many years to enhance tensile strength, wear resistance, elasticity, thermal stability and life span of rubber blends. The reinforcing effectiveness of carbon fillers is well known to be crucially influenced by their structural properties worth mentioning the filler particle size, surface area, degree of agglomeration, porosity and surface chemistry[1,2]. These are, in their turn, substantially dictated by the synthesis and raw materials employed. In recent years, interest has arisen in alternative carbon materials produced from industrial by-products and secondary raw material. This development is motivated by economic and ecological factors, such as cost and waste reduction, as well as the demand for environmentally friendly material alternatives. In this context, secondary raw materials originating from acetylene production by the pyrolysis of natural gas are a potentially interesting yet under-investigated class of functional carbon fillers. This acetylene byproduct secondary raw material (APSR), also known as VSPA in some works, is formed from incomplete carburization and consist of carbon sp3 particles with a complicated and active chemical surface [3].

APSR is distinguished from typical technical carbons by the adsorbed and chemically bonded reaction products of acetylene oligomerisation and oxidation. These surface adsorbed species are composed of oxygen- and hydrogen-containing functional group (referred to as carboxyl, phenolic, quinone and lactone groups), which may play an important role in the interaction between filler particles and polymer matrices. It is believed that the presence of these functional groups will result in better interfacial adhesion, improved dispersion of fillers and provide for a more uniform vulcanization network in elastomeric compounds. The structural and physicochemical characteristics (elemental composition, surface functionalization, dispersity, porosity, and adsorption capacity) of APSR are the lottery in the term of reinforcement. However, in comparison to conventional technical carbons grades, APSR has still not been well characterised with respect to both its surface chemistry and the role of low molecular weight oligomerized fractions lying on the particle surface. These properties are important in order to judge the applicability of APSR as an efficient filler in elastomer formulations [4,5].

Elemental analysis, infrared and nuclear magnetic resonance spectroscopy, electron paramagnetic resonance spectroscopy, and adsorption studies are needed for a complete APSR characterization. These techniques can be used to determine surface functional groups, specific surface area and chemical activity as well as reactivity towards polymer matrices. Analysis in comparison to industrial carbon black grades will also allow an objective assessment of its benefits and disadvantages. Thus, the research on APSR as carbon filler is significant both scientific and application value. Scientifically, it offers insight into the structure–property relationship of functionalized carbon materials. In a technical sense, it introduces new prospects for the application of industrial waste products as effective reinforcing fillers in elastomer technology. The objective of the present study is to carry out systematic analysis of APSR in terms of its structural, physicochemical and functional properties for prospective application as an active filler that could enhance mechanical and technological performance parameters of composite elastomeric mater.

Methodology: The object of the study was the acetylene production secondary raw material (APSR), formed during the pyrolytic decomposition of natural gas. This material represents a complex mixture of carbon particles with a functionalized surface, on which products of incomplete acetylene carbonization are adsorbed. To investigate the structural, physicochemical properties of APSR, a set of methods was employed aimed at determining the elemental composition, particle morphology, the nature of surface functional groups, and their influence on the physical properties.

The research methods included:

1. Elemental Analysis. A quantitative analysis was carried out to determine the content of carbon, hydrogen, oxygen, sulfur, and ash. The aim of this stage was to assess the degree of carbon saturation in APSR and the influence of residual elements on its physicochemical properties, as well as to perform a comparative analysis with standard technical carbons T 900, P 701, P 705, and P 803, which are used in industry as fillers for elastomeric materials.

2. FTIR and NMR Spectroscopy. FTIR spectroscopy was used to identify functional groups on the surface of the carbon particles (carboxyl, phenolic, quinone, and lactone groups), while NMR spectroscopy was employed to confirm the presence of aromatic structures and substituted derivatives. These methods allowed for the assessment of the chemical activity of APSR and its potential ability to interact with the polymer matrix.

3. Determination of Specific Surface Area and Adsorption Characteristics. The specific surface area of APSR was measured using nitrogen, phenol, and CTAB adsorption methods, which allow for the assessment of both the total surface area and the accessibility of active sites. Additionally, the iodine number and oil absorption were determined, reflecting the degree of polyconjugation and the porosity of the particles.

4. Measurement of Morphological Characteristics. The average particle diameter, bulk density, and particle size distribution were studied to assess the dispersity and structural uniformity of APSR. These parameters are critically important for predicting the behavior of the filler during the formation of the vulcanization structure in elastomeric compositions.

5. Extraction of Low-Molecular-Weight Oligomer. APSR was subjected to extraction in toluene, which allowed the isolation of a low-molecular-weight oligomer (12–15% of the initial material mass) with a molecular weight ≤1000. This product is characterized by the presence of oxygen-containing functional groups capable of influencing adhesion to the polymer matrix and the formation of interfacial interactions.

6. Electron Paramagnetic Resonance (EPR) Spectroscopy. This was employed to examine the free radicals and paramagnetic centers in the isolated oligomer. The data presented could be useful to comprehend the reactivity nature of APSR when interacting with polymer matrices and possibly its

participation in the vulcanization processes.

The comparison with commercially available technical carbons (T 900, P 701, P 705 and P 803) was performed in order to assess the specific nature of APSR: dispersity; surface functionalization; chemical reactivity and adsorption properties. This makes it possible to reveal the propensities of polydisperse filler (raw material of acetylene synthesis) as a competent component for composite elastomeric materials.

Result:

Elemental Composition of VSPA

In the creation of composite elastomeric materials, carbon fillers play a significant role, and their structure and properties are largely determined by the methods of their synthesis [7,8,9]. The study of the structural, physicochemical properties of the secondary raw material from acetylene production (VSPA) showed that its composition approaches that of certain grades of well-known technical carbons (Table 1).

Table 1. Elemental composition of acetylene production residue and selected grades of technical carbon.

Parameter name	**Content,%**				
	Secondary raw materials of acetylene production	**T 900**	**P 701**	**P 705**	**P 803**
Carbon	86-90	96-99	96-98	96-98	97-99
Hydrogen	3-4	0,3-0,5	0,4-0,6	0,6-0,8	0,4-0,6
Oxygen	6-7	0,1-0,2	0,3-0,5	0,3-0,5	0,1-0,2
Sulfur	-	0,1	0,3	0,3	0,2
Ash content	0,8-0,9	0,1-0,2	0,4-0,6	0,4-0,5	0,4-0,5

Extraction of low molecular weight oligomer

Extraction of LSA in toluene allowed for the extraction of 12-15% of the low molecular weight oligomer ($M \leq 1000$) on the particle surface. This oligomer contains functional oxygen-containing groups that influence the adhesion to the polymer matrix and the formation of interfacial interaction (Table 2).

Table 2. Elemental composition of the extract.

Name of indicators	**Content, %**
Color	Black
Carboxyl	26
Phenol	14
Quinone	33
Lactone	27

IR and PMR spectroscopy

The IR spectra of the extracted oligomer revealed bands characteristic of the products of thermal cyclization and oligomerization of acetylene with the formula $C_{54}H_{40}O$. PMR spectra showed proton signals at $\delta = 6.85$; 6.70; 7.10 m.u., which corresponds to aromatic structures and their substituted derivatives [10,11].

Table 3. Oligomer ICS Results.

v.k. C=O	v.k. C-H	v.k. C-H	v.k. C=C
at 1710 sm $^{-1}$ at 1730 sm $^{-1}$	Aromatic ring at 3050 см $^{-1}$	Methylene and methyl groups at 2860, 2930, 2960, 2975 sm $^{-1}$	at 1500-1600 sm $^{-1}$

The extracted oligomer produced a narrow single EPR signal with a concentration of $\sim 1\times 10^{14}$ spins/g and a g-factor close to a free electron, indicating the presence of paramagnetic centers.

Physical characteristics of VSPA

Table 4. Comparison of the main physical characteristics of WPA and some technical carbons.

Name of indicator	MU	Technical carbon grade			
		T 900	P 701	P 705	P 803
Specific conditional surface area, m^2/g	19-24	12-16	33-39	20-26	13-19
STAB adsorption specific surface area, m^2/g	57-60	25-30	45-50	38-44	35-40
Specific surface area for phenol adsorption, m^2/g	75-85	10-13	30-35	16-25	12-20
Specific surface area for nitrogen adsorption, m^2/g	85-90	12-15	32-38	18-25	10-20
Iodine number, mg/g	100-110	16-20	34-40	24-28	19-23
Dibu-tyl phthalate absorption, ml/100g	170-180	40-50	60-70	105-115	75-90
Absorption of linseed oil, ml/100 g	165-170	3540	6065	90-100	65-80
pH of aqueous suspension	6-8	6-8	9-11	7,5-9,5	7,5-9,5
Mass loss at 378 K, %	0,4-0,8	0,0-0,4	0,0-0,35	0,0-0,5	0,0-0,5
Specific bulk density, g/cm^3	1,76-1,78	1,88-1,95	1,75-1,78	1,80-1,84	1,81-1,84
Average particle diameter, Nm	45-70	250-300	85-100	888-110	155-210
Mass fraction of residue on the sieve, % 05 K	0,004	0,0008	0,0008	0,0008	0,001
0,14 К	0,003	0,02	0,01	0,01	0,1
0045 К	0,03	0,08	0,08	0,08	0,1

The table presents a comparative characterization of the main physical and adsorption properties of acetylene production secondary raw material (VSPA) and technical carbon grades T 900, P 701, P 705, and P 803. The data indicate that VSPA is distinguished by high particle dispersity, a well-developed specific surface area, and elevated iodine number and oil absorption values, reflecting increased surface roughness and functional activity. The relatively small average particle size and favorable adsorption characteristics of VSPA suggest its strong potential as an active reinforcing filler in composite elastomeric materials.

Discussion: The table data show that LSA has a high dispersity of particles, a developed surface area, and a large number of functional groups. High values of the iodine number and oil absorption indicate surface roughness and the presence of polysubstituted systems. During the formation of WPA, the products of incomplete carbonization of acetylene are adsorbed or chemically bound to its partially oxidized surface[12,13].

VSPA can be considered as soot particles enclosed in a microencapsulated polymer-oligomeric shell with oxygen-containing functional groups. Such a structure ensures:

Improvement of adhesion to the polymer matrix;

Uniform dispersion and formation of a volcanization network;

Improving the operational properties of rubber products [14,15].

Conclusion: This study has shown that secondary material material from acetylene (VSPA) have a specific set of structural, physicochemical and surface properties, which distinguish this material from the accepted grades of technical carbon used in rubber compounds. The VSPA elementary analysis results demonstrated that VSPA had higher oxygen and hydrogen contents than common carbon black, suggesting its surface is partially oxidized and chemically active. This aspect would be an important factor in the behavior of filler particles in polymer matrix. Comprehensive surface area and adsorption studies indicated that VSPA possessed facile specific surface area (SSA) and high capacity of adsorption, due to its notable iodine number and oil absorption. These parameters suggest high surface roughness, excellent polyconjugation degree and availability of active site at the particle surface. In addition,according to the morphological analysis,VSPA was comprised of quite well-separated particles withsmaller average diameters which would contribute to uniform dispersion of filler in elastomers.

The separation of a low-molecular-weight oligomer fraction from VSPA particle surface also contributed to the understanding of its chemical activity. The resulting oligomer, which makes up 12–15 wt. % of the material as carboxyl- and phenolic-, quinone-, lactonic groups. Spectroscopic investigations showed the aromatic structures and oxygen-containing functional groups and EPR analysis revealed production of some paramagnetic centers. These characteristics altogether indicate an increased capacity of VSPA to take part in interphase interactions with elastomeric matrices. According to the above results, VSPA can be defined as carbon particles covered by a polymer–oligomer shell and functionalized with groups. Making the structure in this way helps to enhance the adhesion of filler and polymer, thus making it easier for dispersion, forming a more stable vulcanization structure. Therefore, it can be anticipated that rubber articles are satisfactory in practical service and dynamic properties by means of VSPA used as an active carbon black filler. In conclusion the examined acetylene production by-product has an innovative potential as a new active filler for elastomeric composites. The characteristic of the high dispersity and well-developed surface area as well as chemically active functional groups endow VSPA with great potential to modify structure and properties of elastomeric composites, which also not only provides a rational integration pathway of industrial by-product but also further compensates the stretchingness loss caused in rubber processing.

References

[1] A. Kh. Yusupbekov, A. Ibadullaev, T. R. Abdurashidov, and K. S. Akhmedov, “Acoustic phenomena and interaction in shear flows over compliant and vibrating surfaces,” in Proc. Int. Symp. on Flow-Induced Vibration and Noise, vol. 6, Chemical Technology, Doklady, 1988, no. 301–3, pp. 79–80.

[2] A. Ibadullaev, A. Kh. Yusupbekov, V. A. Gorbunov, and T. R. Abdurashidov, “Reactivity of a secondary carbonaceous raw material with respect to carbon dioxide,” Journal of Applied Chemistry of the USSR, vol. 59, no. 11, pt. 2, pp. 2387–2389, 1986.

[3] B. B. Yoqubov, A. Ibadullaev, D. Q. Yoqubova, and E. U. Teshabaeva, “Prospects and development of research of composite elastomer materials,” Journal of Siberian Federal University. Chemistry, vol. 14, no. 4, pp. 464–476, 2021, doi: 10.17516/1998-2836-0255.

[4] V. M. Goldshtein, Ed., Intensifikatsiya proizvodstva tekhnicheskogo ugleroda. Moscow, USSR: TsNIITE Neftekhim, 1983, 96 p.

[5] V. F. Surovikin, Razvitie i intensifikatsiya pechnogo protsessa proizvodstva tekhnicheskogo ugleroda. Moscow, USSR: TsNIITE Neftekhim, 1976, 65 p.

[6] A. Ibadullaev, A. Kh. Yusupbekov, T. R. Abdurashidov, and V. A. Gorbunov, “Electron-microscopic investigation of the structure of carbon-containing secondary raw materials,” Doklady Akademii Nauk UzSSR, no. 7, pp. 43–45, 1985.

[7] A. Ibadullaev, A. Kh. Yusupbekov, T. R. Abdurashidov, and V. N. Babyuk, “X-ray structural analysis of carbon-containing secondary raw materials,” Doklady Akademii Nauk UzSSR, no. 11, pp. 32–33, 1985.

[8] D. D. Han (Chang Dae Han), Rheology in Polymer Processing, G. V. Vinogradov and M. L. Fridman, Eds., Trans. from English. Moscow–Leningrad, USSR: Khimiya, 1979, 396 p.

[9] V. I. Lusenkov, M. L. Uralskiy, R. A. Gorelik, and A. M. Bukanov, “Methodological features of evaluating technological properties of elastomers using the Brabender Plastograph,” Kauchuk i Rezina, no. 10, pp. 60–63, 1980.

[10] R. S. Onifer, “Discovering the keys to processing better rubber components with the C. W. Brabender Plasti-Corder,” Rubber Age, vol. 98, no. 8, pp. 51–60, 1966.

[11] P. R. Van Buskirk, S. B. Turetski, and P. F. Gunberg, “Practical parameters for mixing,” Rubber Chemistry and Technology, vol. 48, no. 4, pp. 577–591, 1975; vol. 49, no. 1, pp. 1–11, 1996.

[12] M. L. Studebaker and J. R. Beatty, “Mixing factors that affect raw stock,” Rubber Age, vol. 108, no. 5, pp. 21–27, 1996; no. 6, pp. 21–28, 1996.

[13] D. I. Nigmatova, A. S. Ibadullaev, and Sh. I. Mamaev, “Investigation of the influence of ingredients on the vulcanization process of elastomer compositions,” 2023.

[14] A. Ibadullaev, D. Nigmatova, and E. Teshabaeva, “Radiation resistance of filled elastomer compositions,” IOP Conference Series: Earth and Environmental Science, vol. 808, no. 1, 2021.

[15] A. Ibadullayev, E. Teshabayeva, B. Kakharov, and D. Nigmatova, “Composite elastomeric materials filled with modified mineral fillers,” E3S Web of Conferences, vol. 264, p. 05006, 2021.