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INVESTIGATION OF THE DISPERSED-PHASE DISTRIBUTION OF ORGANOCHLORINE PESTICIDES, POLYCHLORINATED BIPHENYLS AND POLYCYCLIC AROMATIC HYDROCARBONS IN NATURAL WATER SYSTEMS

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Abstract. The article analyzes the patterns of the dispersed-phase distribution of organic ecotoxicants, namely organochlorine pesticides (OCPs), polychlorinated biphenyls (PCBs), and polycyclic aromatic hydrocarbons (PAHs), in natural water systems. The relationship between the dispersed-phase distribution of individual OCPs, PCBs, and PAHs and the logarithm of the octanol-water partition coefficient log $K_{o/w}$ (hydrophobicity coefficient) was established. It was shown that the water-soluble part of individual organic ecotoxicants decreases with an increase in their hydrophobicity coefficient. Eight of the given eleven correlations are clear, significant and reliable. The influence of the characteristics of the water system on the dispersed-phase distribution of organic ecotoxicants was also investigated. It was shown that the total water-soluble part of OCPs, PCBs, and PAHs decreases with an increase in the chemical oxygen demand (COD), biological oxygen demand (BOD), and the total concentration of heavy metals (Cr, Ni, Cu, Mn, Zn, Cd, Pb). Four of the nine relevant correlations are clear, significant, and reliable.

Keywords: OCPs, PCBs, PAHs, dispersed-phase distribution, coefficient of hydrophobicity, COD, BOD.

1. Introduction

Organochlorine pesticides (OCPs), polychlorinated biphenyls (PCBs), and polycyclic aromatic hydrocarbons (PAHs) are characterized by extremely high toxicity, persistence in the environment and bioavailability for living organisms. They can have carcinogenic, mutagenic, teratogenic, hepatotoxic and other effects on the human body.[1]

In order to protect public health and the environment, the UN has adopted a number of important decisions to limit the production and use of these highly toxic chemicals. Thus, at the UN conference on May 22, 2001, the Stockholm Convention on Persistent Organic Pollutants (POPs) was approved.[2] The initial list of POPs included compounds of the following classes: OCPs, PCBs, polychlorinated dibenzo-*p*-dioxins, and polychlorinated dibenzofurans. One of the Convention's requirements is the monitoring of individual compounds of these classes in the environment, in particular in natural water systems. The list of POPs is expanding, and today PAHs are candidates for inclusion in this directory.

The results of the complex long-term studies on the determination of the total concentration of organic ecotoxicants OCPs, PCBs, and PAHs in the surface water of the Dnieper River are presented in papers.[1,3,4]

According to their physicochemical properties, OCPs, PCBs, and PAHs are nonpolar, semi-volatile, hydrophobic organic compounds.[1] In this regard, in natural water systems, they are located in the following physical forms: in a soluble state; in a bound state with suspended particles; in sorbed and solubilized states with organic compounds of natural and anthropogenic origin. Physical forms of organic xenobiotics differ in the degree of bioavailability. Therefore, to assess the ecological threat, it is important to determine its distribution among different forms, in addition to the integral concentration of the toxicant in water.

Milyukin and co-workers[5] analyzed and summarized the results of the study of the dispersed-phase distribution of OCPs, PCBs, and PAHs between the aqueous phase (true water-soluble state), the fine fraction of suspended particles (particle size >0.45 and <16–24 μm) and the coarse fraction of suspended particles (>16–24 μm) in the surface water of the Dnieper River. It was found that compounds of these classes are located predominantly in the bound state with suspended particles. The water-soluble parts of OCPs, PCBs, and PAHs are on average

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32, 42, and 44%, respectively. The average proportions of OCPs, PCBs and PAHs in coarse and fine fractions of suspended particles are 50, 34, 37% and 18, 24, 19%, respectively.

Similar studies to determine the dispersed-phase distribution of organic ecotoxicants have been performed for other natural water systems. It was found that in the water of the Tiber River (Italy),[6] Pearl River Delta (China),[7] and Yangtze River (China),[8,9] the water-soluble parts of OCPs and PCBs were 54, 75, 52% and 16, 69, 84%, respectively. PAHs in the surface water of the Tiber River[10] and Daliao River (China)[11] were located mainly in the bound state with suspended particles. Their water-soluble parts were 21 and 16%, respectively.

From these data, it can be concluded that in natural water systems, a significant proportion of organic xenobiotics is located in a bound state with suspended particles. At the same time, it was found that the dispersed-phase distribution of individual compounds of these classes differs significantly from each other. For example, in the surface water of the Dnieper River, PCB congeners with two or three chlorine atoms were located predominantly in a water-soluble state. This is due to the fact that they are less hydrophobic and characterized by relatively high water solubility. The most common tetra-, penta-, and hexa-PCBs were approximately equally distributed between the aqueous and suspended phases, while the hepta-PCBs, due to their high hydrophobicity, bound almost completely with suspended particles.[5] A similar trend has been established for OCPs: less hydrophobic isomers of hexachlorocyclohexane (HCH) are located predominantly in the water-soluble state, and more hydrophobic pesticides of the dichlorodiphenyltrichloromethylmethane (DDT) group are bound with suspended particles. Among the individual PAHs, only naphthalene, which is less hydrophobic, was located mainly in the aqueous phase. The water-soluble parts of other more hydrophobic PAHs did not exceed 28%.

Milyukin and Gorban[12] analyzed the results of the dispersed-phase distribution of OCPs, PCBs, and PAHs in the water of various river systems. The following pattern was established for all studied river systems: the higher the logarithm of the octanol-water partition coefficient log $K_{o/w}$ (hydrophobicity coefficient) of an organic ecotoxicant, the lower its water-soluble fraction. The corresponding dependencies were established and statistically processed. For most cases, reliable and significant correlations were obtained. This implies that the hydrophobicity coefficient of a compound is an important indicator by which its dispersion-phase distribution can be estimated.

The dispersed-phase distribution of hydrophobic organic ecotoxicants (OCPs, PCBs, PAHs), in addition to the hydrophobicity coefficient, is influenced by many natural factors that characterize the water system. These include salinity; alkalinity of water; concentration of suspended particles, their chemical nature and size; pH of the medium; buffering capacity of the natural system; content of natural organic substances (humic and fulvic acids (HFAs), protein-like substances, synthetic surfactants, high molecular weight carbohydrates, algae); concentration of heavy metals; a temperature of the water system, etc.

Various algae have a special influence on the dispersed-phase distribution of organic ecotoxicants in natural water systems. They can release a lot of toxic amines, diamines, and polyamines, which are capable of entering into various secondary reactions to form even more toxic substances. Given that these compounds are excellent complexing agents, they are capable of forming complex conjugates with OCPs, PCBs, and PAHs. As a result, organic ecotoxicants can end up on various dispersed particles.[13]

Petrov *et al.*[14] analyzed data on the abundance and richness of marine diatom species in Balaklava Bay (Black Sea, Crimea) and measured 15 variables: depth, structure, size composition of bottom sediments, Total Organic Carbon (TOC), metals (Zn, Ni, Cu, Pb, Hg, Cd, Cr, Mn), OCPs, PCBs, and PAHs. The results of the analyses showed that the combination of depth, percentage of sand fraction, TOC, OCPs, PCBs, and Hg content had the most significant effect on the structure and diversity of the diatom communities. As a result of this study, it was found that these features allow us to recommend this group as a reliable indicator of eutrophication and anthropogenic pollution in the integrated monitoring of aquatic ecosystems.

The purpose of this study was to establish and analyze the dependence of the dispersed-phase distribution of organic ecotoxicants in the water of the world's river systems on the hydrophobicity coefficient of compounds and on the parameters of the water system itself.

2. Experimental

2.1. Methodology for the determination of organic ecotoxicants

For determination of the dispersed-phase distribution of OCPs, PCBs, and PAHs the methodology was developed and applied for analysis of surface water from the Dnieper River.

The concentrations of the following compounds were determined: OCPs – α-, β-, γ-hexachlorocyclohexanes (HCH), hexachlorobenzene (HCB), heptachlor, aldrin, 4,4'-dichlorodiphenyldichloroethylene (DDE), 4,4'-dichlorodiphenyldichloroethane (DDD), 4,4'-dichlorodiphenyltrichloroethane (DDT); PCBs – 2,4'-di-

(number 8); 2,2',5-tri- (18); 2,4,4'-tri- (28); 2,4',5-tri- (31); 2,2′,5,5′-tetra- (52); 2,2',4,5'-tetra- (49); 2,2',3,5'-tetra- (44); 2,3',4,4'-tetra- (66); 2,2',4,5,5'-penta- (101); 2,2',4,4',5-penta- (99); 2,3,3',4',6-penta- (110); 2,2',3,4',5',6-hexa- (149); 2,2',3,5,5',6-hexa- (151); 2,3',4,4',5-penta- (118); 2,2',4,4',5,5'-hexa- (153); 2,3,3',4,4'-penta- (105); 2,2',3,4,4',5'-hexa- (138); 2,2',3,4',5,5',6-hepta- (187); 2,2',3,4,4',5',6-hepta- (183); 2,2',3,3',4,4'-hexa- (128); 2,2',3,3',4,5,6'-hepta- (174); 2,2',3,3',4,5',6'-hepta- (177); 2,2',3,4,4',5,5'-hepta- (180); 2,2',3,3',4,4',5-hepta- (170); 2,2',3,3',4,5,5',6'-octa- (199); 2,2',3,3',4,4',5,6-octa- (195); 2,2',3,3',4,4',5,5'-octa- (194); 2,2',3,3',4,4',5,5',6-nona- (206); 2,2',3,3',4,4',5,5', 6,6'-deca- (209); PAHs – naphthalene, acenaphthylene, acenaphthene, phenanthrene, anthracene, fluoranthene, pyrene, benzo(a)anthracene, chrysene, benzo(b)fluoranthene, benzo(k)fluoranthene, benzo(a)pyrene, dibenzo(a,h) anthracene, benzo(ghi)perylene, indeno(1,2,3-cd)pyrene.

The methodology of determination of the dispersed-phase distribution of OCPs, PCBs, and PAHs in natural water is schematically presented in Fig. 1. Let's take a look at its stages.

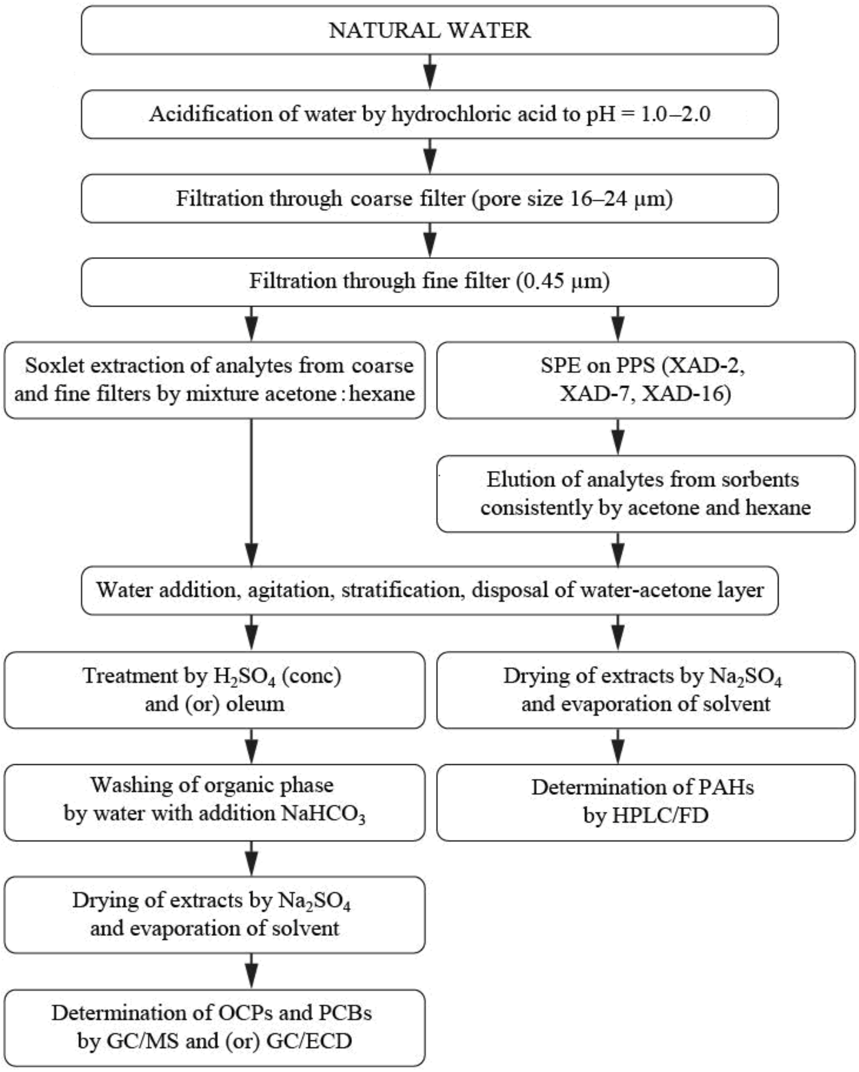

Fig. 1. Scheme of investigation of OCPs, PCBs, and PAHs in the natural water

Sampling was carried out in the Dnieper River at a depth of 0.5–1 m by bathometer. Collected samples were acidified to pH 1.0–2.0 by hydrochloric acid. A specific volume of water was allowed to go sequentially through coarse (pore size 16–24 μm), fine (0.45 μm) filters, and porous polymer sorbents (PPS) as follows XAD-2, XAD-7, and XAD-16.

After filtration, coarse and fine filters were dried to air-dry condition. Then coarse filters were homogenized and placed in the Soxhlet apparatus for extraction of organic compounds. Fine filters were not homogenized, and after drying they were placed in the Soxhlet apparatus for extraction of organic compounds. Extraction of organic compounds from filters was carried out by a mixture of organic solvents acetone:hexane (1:1) in the Soxhlet apparatus for 16 h.

Elution of organic compounds from sorbents XAD-2, XAD-7, and XAD-16 was performed sequentially by acetone and hexane (1:1). To an acetone-hexane solution of analytes, water was added. After intensive agitation and subsequent stratification water-acetone layer was disposed of.

In analyzing OCPs and PCBs, hexane solution was processed by concentrated sulphuric acid and (or) oleum for the disposal of redundant organic substances. The cleared hexane solution was washed with three amounts of MilliQ Water with the addition of sodium hydrogencarbonate (mass concentration – 3%).

After that, a hexane solution of OCPs and PCBs was dried by freshly calcined sodium sulfate and evaporated to a specific volume. An aliquot of the final extract was injected into the gas chromatograph. Identification and determination of OCPs and PCBs were performed by gas chromatography/mass spectrometry (GC/MS) and gas chromatography/electron-capture detection (GC/ECD) respectively to previously developed methodology.[1] For the measurements the following devices were used: GC/MS System (Agilent Technologies, Inc.) in the SCAN and SIM mode on an Agilent GC6890N coupled to MSD5975 Inert XL and Autoinjector 7683B; gas chromatography with an electron capture detector (GC/ECD) on HP GC5890 Series II with a single ECD.

In analyzing PAHs after disposal of the water-acetone layer, hexane extract was dried by freshly calcined sodium sulfate and evaporated to a specific volume. An aliquot of the final extract was injected into the liquid chromatograph. Identification and determination of PAHs were performed by high-performance liquid chromatography with fluorescence detection (HPLC/FD). PAH concentrates were analyzed on a Waters Alliance with an E2695 separation module, 2998 photodiode array, and 2475 multiwavelength fluorescent detector.

In monograph,[1] the determination of PAHs is presented in more detail.

2.1.1. GC/MS procedure

OCPs and PCBs were measured by GC/MS System (Agilent Technologies, Inc.) in the SCAN and SIM modes on an Agilent GC6890N coupled to MSD5975 Inert XL and Autoinjector 7683B.

Purified concentrates of OCPs and PCBs with a volume of 1 μL were injected with a Hamilton syringe into the PTV injector of the gas chromatograph without splitting the flow (splitless for 1 min).

Chromatographic conditions in the SCAN and SIM modes: column – HP-5MSI or HP-5MS (5 % phenylmethylsiloxane) (30m×0.25mm×0.25μm); carrier gas – helium, linear rate – 37.0 sm/s, volume rate – 1 mL/min with temperature correction of the carrier gas flow rate; initial pressure at the inlet to the capillary column (in the PTV injector) – 8.23 psi (56 kPa); oven temperature program – from 60 to 160 °C with a heating rate of 25 °C/min, from 160 to 300 °C – 10 °C/min and isothermic period at 300 °C – 5 min (chromatography time – 23 min). The collection of mass spectrometric data began 6 min after the injection of the sample into the gas chromatograph injector (Solvent delay – 6 min).

Mass spectrometric conditions: detector parameters – SCAN or SIM modes at EI (70 eV), mass spectra were recorded with an electron multiplier at a voltage of 0.9–1.4 kV and a pressure of $2 \cdot 10^{-5}$ Pa in the source area ions in the mass range with m/z 34–550 amu. The temperatures of the interface, quadrupole, and ion source are 250, 150–200, and 230 °C, respectively.

The determination of OCPs and PCBs was carried out in the SIM mode with mass selective detection by characteristic ions for these compounds with m/z: 109, 181, 219 (α-, β-, γ-, δ-HCH), 100, 135, 272 (heptachlor), 66, 220, 263 (aldrin), 176, 246, 248 (4,4'-DDE), 165, 235, 237 (4,4'-DDD, 4,4'-DDT) and 256, 258, 260 (trichloro-), 290, 292, 294 (tetrachloro-), 324, 326, 328 (pentachloro-), 358, 360, 362 (hexachloro-), 392, 394, 396 (heptachloro-), 426, 428, 430 (octachloro-), 460, 462, 464 (nonachloro-).

2.1.2. GC/ECD procedure

OCPs and PCBs were determined by gas chromatography with an electron capture detector (GC/ECD) on HP GC5890 Series II with a single detector. The sample of organic contaminants (1 μL) was injected into an injector of the chromatograph splitless by Hamilton syringe. Chromatography conditions: carrier gas – nitrogen; inlet pressure – 50 kPa; oven temperature program – from 60 to 270 °C, rate – 8 °C/min, then – isothermally at 270 °C for 15 min; column – HP-5 (25m×0.25mm×0.32μm). Makeup gas – nitrogen; inlet pressure – 100 kPa; rate – 40 mL/min; anode purge – 4 mL/min. Injector – 280 °C. Detector – 300 °C.

2.1.3. HPLC/FD procedure

Identification and determination of PAHs in the obtained concentrates was performed by high-performance liquid chromatography by fluorescence detection (HPLC/FD). PAH concentrates were analyzed on a Waters Alliance with an E2695 separation module, 2998 photodiode arrow, and 2475 multiwavelength fluorescent detector. Parameters: Merck column 150433 – 250×4.6 mm; sorbent – LiChrosorb RP-18, 5 µm; injected (autoinjector) volume – 50–100 µL; mobile phase – A (CH_3CN/H_2O, v/v 4:5), B (CH_3CN); pump gradient – from 100 % A to 100 % B, 50 min; then B – 10 min; temperature – 25 °C. Detection was carried out simultaneously on 4 channels with the following parameters: A – $\lambda_{ex} = 256$, $\lambda_{em} = 370$; B – $\lambda_{ex} = 260$, $\lambda_{em} = 420$; C – $\lambda_{ex} =$ $= 275$, $\lambda_{em} = 420$; D – $\lambda_{ex} = 290$, $\lambda_{em} = 430$ nm; detector attenuation (photomultiplier gain) – 64; the polarity – positive; output signal – emission. The MDLs of this procedure for PAHs is 0.01 ng/L at the enrichment factor $(1.4–2.8)\cdot10^3$.

2.2. Method for the determination of heavy metals

Before analysis, water samples were filtered (0.45 µm nylon filters) and acidified with 65% nitric acid (super pure 99.99%, 5 mL/L water sample). Heavy metals (Zn, Ni, Cu, Pb, Cd, Cr, Mn) were analyzed in duplicate using inductively coupled plasma mass spectrometry (ICP/MS), on an Agilent 7500 CE. Trace metal determination in water samples was performed according to the International Standards: ISO 17294-1:2004, and ISO 17294-2:2003 for 62 elements.

Pre-filtration resulted in two types of samples used in the investigation: total fraction and fraction <0.45 µm. For digestions, filters were dried (70–80 °C), and finely ground in agate mortgage. These samples were then processed using a microwave-assisted digestion system (Speed Wave MWS-2, Berghof Products Instruments GmbH) in closed digestion vessels containing $HNO_3 : HCl$ (3 : 1) for 30 min. Following extraction, digests were filtered through 0.45 µm polyvinylchloride membranes, diluted with deionized water to 10 mL, and stored at room temperature until analysis by ICP/MS. Method detection limits (MDLs) for the metals ranged from 0.01 to 0.1 µg/L.

The device was calibrated to determine metals using solutions containing certain concentrations, namely: 0.1, 1.0, 10.0, 50.0, and 100.0 µg/L. These solutions were prepared by diluting the stock ICP Multi Element Standard Solution XXI CertiPUR® 2.74473.0100 from Merk with a concentration of each element of 10 mg/L with nitric acid (3–5 wt%).

3. Result and Discussion

3.1. Dependence of the dispersed-phase distribution of organic ecotoxicants on their hydrophobicity coefficient

For a number of aquatic systems, the relationship between the water-soluble fraction of OCPs, PCBs, and PAHs and their hydrophobicity coefficient was analyzed in paper.[12] The results on the dispersed-phase distribution of organic ecotoxicants in other aquatic systems were used in this study.

Thus, the dependence of the water-soluble fraction of individual OCPs on the hydrophobicity coefficient in the surface water of the Dnieper River[5] was compared with the corresponding dependencies for other natural water systems, namely the Elbe River (Germany),[15] the Xiangshan Bay (East China Sea)[16] and the Ria Formosa Lagoon (south of Portugal).[17] The corresponding graphs of dependencies are shown in Fig. 2. The results were statistically processed using Pearson's correlation analysis by the Statistical Package for the Social Sciences version 19 (SPSS, Inc., IBM Company, Chicago, IL), in particular, the correlation coefficient (r) and the probability criterion (p) were calculated. As you know, a correlation is considered reliable if the condition $p < 0.05$ is met.

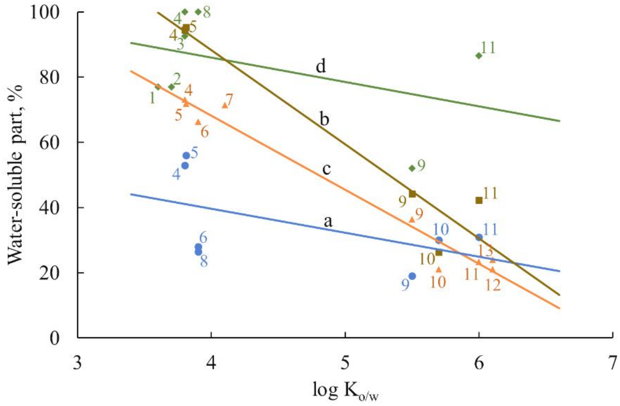

Fig. 2. Dependence of the average value of the water-soluble part of individual OCPs on their hydrophobicity coefficient log $K_{o/w}$ in the waters of the Dnieper River (a), r = -0.5319, p = 0.2191; the Elbe River (b), r = -0.9622, p = 0.0088; the Xiangshan Bay (c), r = -0.9854, p = 0.00001; the Ria Formosa Lagoon (d), r = -0.4362, p = 0.3278. The names of OCPs are indicated by numerals: 1 – dieldrin; 2 – β-endosulfan; 3 – α-endosulfan; 4 – γ-HCH; 5 – α-HCH; 6 – β-HCH; 7 – σ-HCH; 8 – heptachlor; 9 – 4,4'-DDD; 10 – 4,4'-DDE; 11 – 4,4'-DDT; 12 – 2,4'-DDT; 13 – 2,4'-DDD

As can be seen from Fig. 2, in all of the above water systems, the water-soluble part of individual OCPs decreases with an increase in the logarithm of the octanol-water partition coefficient log $K_{o/w}$. At the same time, no clear reliable correlation was established between the Dnieper River and the Ria Formosa Lagoon. The correlation coefficients in these cases are low. There is only a slight decrease in the water-soluble part of individual OCPs with an increase in their hydrophobicity coefficient. The water-soluble parts of individual OCPs in the water of the Ria Formosa Lagoon were 52–100 % and were much higher than in the water of the Dnieper River, which ranged from 19 to 56 %.

In the cases of the Elbe River and the Xiangshan Bay, the HCH pesticides were almost entirely located in a water-soluble state, while DDT, DDE, and DDD were predominantly associated with suspended particles. In general, the above correlations are clear and reliable. Thus, in these aqueous systems, the dispersed-phase distribution of individual OCPs is determined mainly by the value of their hydrophobicity coefficient.

Fig. 3 shows the dependence of the water-soluble part of individual PCB congeners on the hydrophobicity coefficient for different water systems. For the Dnieper River[5] and the Elbe River,[15] clear, reliable, significant antibatic correlations were found between the water-soluble part of individual PCBs and the log $K_{o/w}$ value. This is due to the fact that these river systems are flat with a slow and calm flow and are close to each other in terms of water quality parameters. For example, in the Dnieper River water, the values of chemical oxygen demand (COD), the oxidizing agent is potassium permanganate, and biological oxygen demand (BOD) were 10.95 and 4.35 mgO_2/L, respectively. In the water of the Elbe River, the values of these parameters were 15.0 and 4.8 mgO_2/dm^3, respectively.[18] This indicates approximately the same content of organic matter in the water of these water systems. Undoubtedly, this indicator has a significant impact on the dispersed-phase distribution of PCBs in water systems, which will be discussed further.

The same trend is observed for the water of the rivers in Shanghai (China).[19] This correlation is reliable and significant.

Similar results were obtained for the dispersed-phase distribution of PAHs. Fig. 4 shows the dependence of the water-soluble fraction of individual PAHs on their hydrophobicity coefficient for the Dnieper River,[5] the Elbe River,[15] the Pearl River Delta,[20] and the Danube River Delta (Romania).[21]

For the Dnieper River and the Elbe Rivers, the results are almost identical. These correlations are clear and reliable. In these water systems, only naphthalene, which differs significantly from other compounds in its properties, is almost completely water-soluble. The water-soluble fractions of other PAHs (starting with anthracene) are approximately equal and do not exceed 30%.

In the water of the Pearl River Delta, individual PAHs were approximately equally distributed between the aqueous and dispersed phases but the graph shows a tendency to decrease the water-soluble fraction with an increase in the hydrophobicity coefficient. This correlation is reliable and significant.

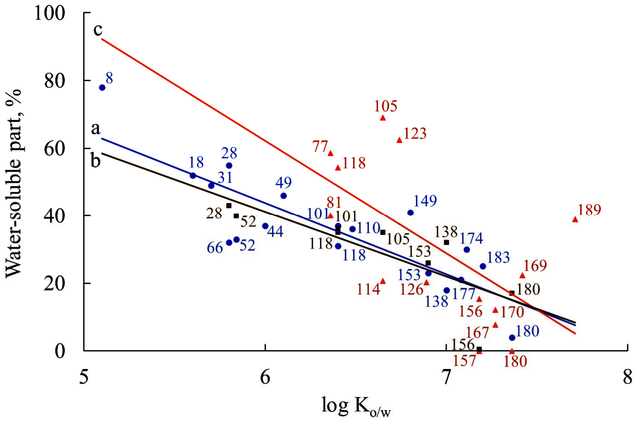

Fig. 3. Dependence of the average value of the water-soluble part of individual PCBs on their hydrophobicity coefficient log $K_{o/w}$ in the waters of the Dnieper River (a), r = -0.8463, p = 0.00001; the Elbe River (b), r = -0.7984, p = 0.0099; the rivers in Shanghai (c), r = -0.6213, p = 0.0177. The numerals indicate the numbers of PCB congeners

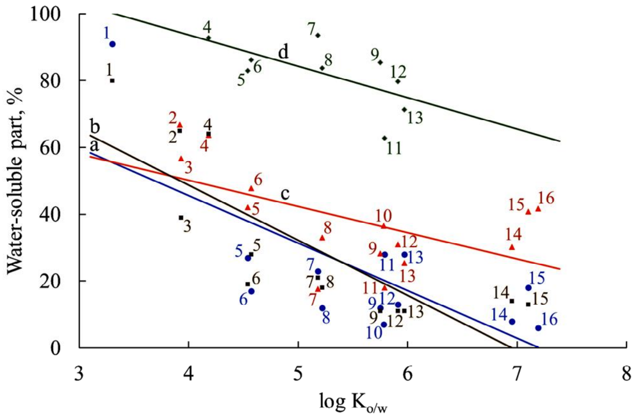

Fig. 4. Dependence of the average value of the water-soluble part of individual PAHs on their hydrophobicity coefficient log $K_{o/w}$ in the waters of the Dnieper River (a), r = -0.7142, p = 0.0061; the Elbe River (b), r = -0.8103, p = 0.0008; the Pearl River Delta, (c), r = -0.5706, p = 0.0263; the Danube River Delta (d), r = -0.6402, p = 0.0633. The names of PAHs are indicated by numerals: 1 – naphthalene, 2 – acenaphthene, 3 – acenaphthylene, 4 – fluorene, 5 – anthracene, 6 – phenanthrene, 7 – pyrene, 8 – fluoranthene, 9 – benzo(b)fluoranthene, 10 – benzo(k)fluoranthene, 11 – chrysene, 12 – benzo(a)anthracene, 13 – benzo(a)pyrene, 14 – indeno(1,2,3-cd)pyrene, 15 – benzo(g,h,i)perylene, 16 – dibenzo(a,h)anthracene

In the case of the Danube River Delta, the water-soluble parts of individual PAHs are significantly higher than in other water systems. They were in the range of 62.7–93.6%. No clear reliable correlation was found for this water system.

Thus, in all of the above cases, a decrease in the water-soluble fraction of individual PCBs, PCBs, and PAHs is observed with an increase in their hydrophobicity coefficient. For some water systems, in particular for the Dnieper River and the Elbe River, significant, clear and reliable correlations were found, which practically coincided with each other. The results obtained indicate that the hydrophobicity coefficient of individual organic ecotoxicants is an important indicator that can be used to assess their dispersed-phase distribution. However, if this factor affecting the distribution were the only one, all correlations would be clear and reliable and would coincide with each other.

The dispersed-phase distribution of organic ecotoxicants is influenced not only by factors that characterize individual substances but also by the properties of the natural water system.

In fact, the dispersed-phase distribution of OCPs, PCBs, and PAHs is influenced by many natural factors, including salinity, alkalinity of water, concentration of suspended particles, their chemical nature and size, pH of the medium, buffering capacity of the natural system, content of natural organic substances (HFAs, protein-like substances, synthetic surfactants, high molecular weight carbohydrates), temperature of the water system, etc. The influence of some parameters of the water system on the dispersed-phase distribution of organic ecotoxicants is analyzed further.

3.2. Dependence of the dispersed-phase distribution of organic ecotoxicants on the parameters of the water system

The relationship between the dispersed-phase distribution of OCPs, PCBs, and PAHs in water and such indicators as COD (oxidizing agent is potassium permanganate), BOD and the sum of heavy metals (Cr, Ni, Cu, Mn, Zn, Cd, Pb) was established and analyzed. These data were obtained from the literature and are presented in Table. In the case of the Dnieper River, water quality parameters were obtained using the methods described in paper.[22] The specified COD and BOD values coincide with the values given for Ukrainian water systems in paper.[23]

Fig. 5 shows the dependence of the total water-soluble fraction of OCPs, PCBs, and PAHs on the COD value in water. It is known that COD is an indicator of the content of organic compounds in water. It has been established that the water-soluble fraction of organic ecotoxicants in water decreases with an increase in the content of organic compounds in water. The most clear and reliable correlation was established for PCBs. In the case of OCPs and PAHs, the correlations are less clear and unreliable.

The above correlations can be explained by the fact that organic ecotoxicants are characterized by a high affinity for organic substances, so in water systems they adsorb mainly on suspended organic particles, including colloidal and high molecular weight particles. If there are few organic compounds in the water, then OCPs, PCBs, and PAHs have nothing to bind with and are mainly located in a water-soluble state. On the contrary, organic ecotoxicants are predominantly bound with suspended particles.

Values of COD, BOD, total heavy metals and total water-soluble part of PCBs, OCPs and PAHs in the water systems

Name of water system	COD, mg/L	BOD, mg/L	Sum of heavy metals, μg/L	Total water-soluble part, %		
				OCPs	PCBs	PAHs
Dnieper River	10.95[22]	4.35[22]	119.5[22]	32.0[5]	42.0[5]	44.0[5]
Elbe River	15.0[18]	4.8[18]	405.1[24]	39.5[15]	29.4[15]	30.3[15]
Pearl River Delta	4.41[25]	3.64[25]	70.3[26]	74.5[7]	69.0[7]	33.1[20]
Tiber River		5.06[27]	732.6[28]	53.8[6]	15.6[6]	21.3[10]
Shanghai Rivers	6.97[29]		79.2[30]		45.9[19]	37.4[31]
Daliao River	8.56[32]	6.77[32]		59.5[33]		15.7[11]
Yangtze River Delta	2.7[34]	1.27[35]	11.5[36]		83.8[9]	
Danube River Delta	3.09[37]	1.76[37]				85.3[21]
Xiangshan Bay	0.97[38]		23.0[39]	51.8[16]		
Ria Formosa Lagoon		2.7[40]		76.0[17]		
Jinjiang River	8.5[41]			36.0[42]		

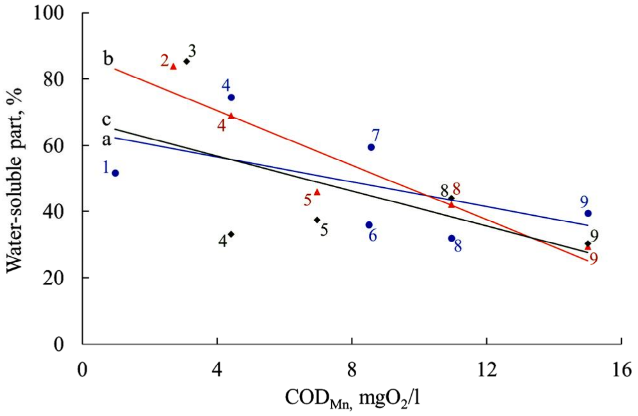

Fig. 5. Dependence of the average value of the water-soluble part of OCPs (a), r = -0.5735, p = 0.2341; PCBs (b), r = -0.9374, p = 0.0186; PAHs (c), r = -0.5745, p = 0.3110, on COD, in natural water, oxidizing agent is potassium permanganate. The names of water systems are indicated by numerals: 1 – the Xiangshan Bay, 2 – the Yangtze River Delta, 3 – the Danube River Delta, 4 – the Pearl River Delta, 5 – the rivers in Shanghai, 6 – the Jinjiang River, 7 – the Daliao River, 8 – the Dnieper River, 9 – the Elbe River

It follows that in such water systems, the main carrier and source of OCPs, PCBs and PAHs pollution is suspended organic particles, from where ecotoxicants can either enter and accumulate in sediments or diffuse back into the water phase.

Fig. 6 shows the dependence of the total water-soluble fraction of OCPs, PCBs, and PAHs on the BOD value in water. BOD is one of the important criteria for the level of water pollution, which determines the amount of easily oxidizable organic substances in water. As we can see, there is a similar tendency to a decrease of the water-soluble fraction of organic ecotoxicants with the growth of BOD. In the case of PCBs and PAHs, clear and reliable correlations were installed. The same trend has been established for OCPs, but the correlation has a low coefficient and is not reliable.

Let us consider the dependence of the total water-soluble part of organic ecotoxicants on the total amount of heavy metals (Fig. 7). It is obvious that no correlation was found for OCPs, only a slight decrease in their water-soluble part was observed with an increase in the concentration of heavy metals. For PCBs and PAHs, clear reliable correlations were established.

From these results, it can be concluded that high values of COD, BOD, and total heavy metals indicate a low water-soluble part of OCPs, PCBs, and PAHs. If the water is characterized by low levels of organic compounds and heavy metals, then organic ecotoxicants are mainly located in a water-soluble state. These results can be useful for the design of effective water treatment systems, as well as for assessing the bioavailability of these compounds and the environmental threat they may pose.

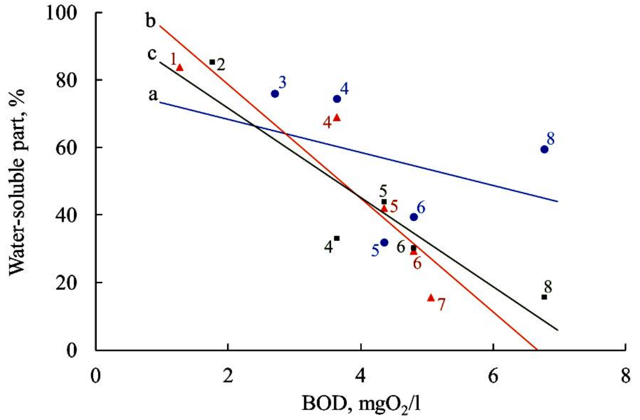

Fig. 6. Dependence of the average value of the water-soluble part of OCPs (a), r = -0.3720, p = 0.5376; PCBs (b), r = -0.9140, p = 0.0299; PAHs (c), r = -0.9107, p = 0.0316, on BOD, in natural water. The names of water systems are indicated by numerals: 1 – the Yangtze River Delta, 2 – the Danube River Delta, 3 – Ria Formosa Lagoon, 4 – the Pearl River Delta, 5 – the Dnieper River, 6 – the Elbe River, 7 – the Tiber River, 8 – the Daliao River

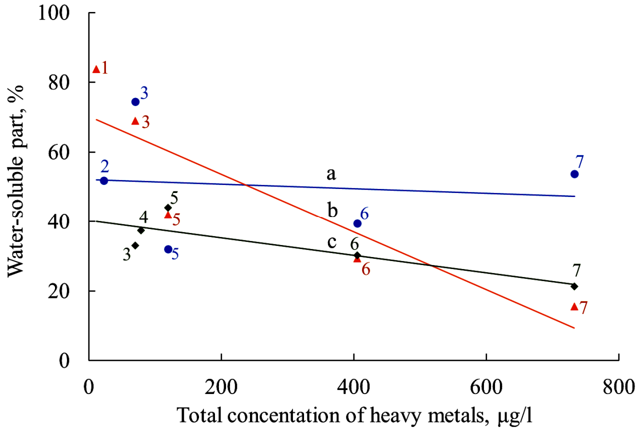

Fig. 7. Dependence of the average value of the water-soluble part of OCPs (a), r = -0.1183, p = 0.8497; PCBs (b), r = -0.8897, p = 0.0433; PAHs (c), r = -0.8567, p = 0.0637, on the total concentration of heavy metals (Cr, Ni, Cu, Mn, Zn, Cd, Pb), in natural water. The names of water systems are indicated by numerals: 1 – the Yangtze River Delta, 2 – the Xiangshan Bay, 3 – the Pearl River Delta, 4 – the rivers in Shanghai, 5 – the Dnieper River, 6 – the Elbe River, 7 – the Tiber River

This work was performed in order to establish correlations between the water-soluble part of the above organic ecotoxicants in different water systems and the coefficient of hydrophobicity log $K_{o/w}$, which characterizes the physicochemical properties of individual compounds, as well as the parameters of COD, BOD and total content of heavy metals that characterize the natural water system.

Using the given correlation dependences it is possible to anticipate the disperse-phase distribution of the mentioned organic ecotoxicants in natural water.

By selecting certain types of coagulants and flocculants and using them for water treatment it is possible to remove a significant part of ecotoxicants sorbed on suspended particles.

OCPs, PCBs, and PAHs are bioavailable compounds capable of bioaccumulation (bioconcentration) along the trophic chain. At the same time, different forms of the compound in natural water (water-soluble form, bound state with suspended fine and coarse particles, etc.) differ in the degree of bioavailability for aquatic organisms. The most accessible form for them is the water-soluble fraction of ecotoxicants, so it poses a significant threat to the ecological state of water systems.

4. Conclusions

Based on the analysis of the experimental material, the dependence of the water-soluble fraction of individual organic ecotoxicants on their hydrophobicity coefficient for different natural water systems was determined. For all cases, there is a tendency to decrease the water-soluble fraction of individual OCPs, PCBs, and PAHs with an increase in the logarithm of the octanol-water partition coefficient log $K_{o/w}$.

Eight of the eleven correlations are significant, clear, and reliable. They are characterized by high correlation coefficients r ranging from -0.571 to -0.985 and low values of the probability criterion p, which were less than 0.05. The results for the Dnieper River and the Elbe River were almost identical. This is due to the fact that these river systems are similar in terms of water quality parameters, in particular the content of organic matter.

The one correlation for PAHs in the natural water of the Danube River Delta also has a high correlation coefficient and a probability criterion approaching 0.05 ($r = -0.6402$, $p = 0.0633$).

The influence of such indicators as COD, BOD, and total heavy metals on the dispersed-phase distribution of organic ecotoxicants in surface water for 11 water systems was also analyzed. It is shown that the total water-soluble fractions of OCPs, PCBs, and PAHs in water decrease with increasing values of COD, BOD, and the sum of heavy metals such as Cr, Ni, Cu, Mn, Zn, Cd, and Pb. The corresponding dependencies were established and statistically processed. Four of nine correlations are significant, clear, and reliable.

The one correlation between the water-soluble part of PAHs in natural water and the total concentration of heavy metals also has a high correlation coefficient and a probability criterion approaching 0.05 ($r = -0.8567$, $p = 0.0637$).

On the basis of the conducted studies, a general trend in the dispersed-phase distribution of individual organic ecotoxicants in water was established. Reliable and significant correlations between the water-soluble part of ecotoxicants and their hydrophobicity coefficient were found for most water systems.

It is also shown that the dispersed-phase distribution of the total amount of organic ecotoxicants in the water system depends on the parameters of the water system itself (COD, BOD, the sum of heavy metals). In some cases, the established correlations are clear and reliable.

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ДОСЛІДЖЕННЯ ДИСПЕРСНО-ФАЗОВОГО РОЗПОДІЛУ ХЛОРОРГАНІЧНИХ ПЕСТИЦИДІВ, ПОЛІХЛОРОВАНИХ БІФЕНІЛІВ І ПОЛІЦИКЛІЧНИХ АРОМАТИЧНИХ ВУГЛЕВОДНІВ У ПРИРОДНИХ ВОДНИХ СИСТЕМАХ

Анотація. *У статті проаналізовано закономірності дисперсно-фазового розподілу органічних екотоксикантів, а саме: хлорорганічних пестицидів (ХОП), поліхлорованих біфенілів (ПХБ) і поліциклічних ароматичних вуглеводнів (ПАВ) – у природних водних системах. Встановлено залежність між дисперсно-фазовим розподілом індивідуальних ХОП, ПХБ та ПАВ і логарифмом константи розподілу в системі октанол/вода log* $K_{o/w}$ *(коефіцієнтом гідрофобності). Показано, що водорозчинна частка індивідуальних органічних екотоксикантів зменшується зі збільшенняи їхнього коефіцієнту гідрофобності. Із одинадцяти наведених кореляцій вісім є чіткими, значимими та достовірними. Також досліджено вплив характеристик водної системи на дисперсно-фазовий розподіл органічних екотоксикантів. Показано, що загальна водорозчинна частка ХОП, ПХБ та ПАВ зменшується зі збільшенням значення хімічного споживання кисню (ХСК), біологічного споживання кисню (БСК) та суми важких металів (Cr, Ni, Cu, Mn, Zn, Cd, Pb). Із дев'яти відповідних кореляцій чотири є чіткими, значимими та достовірними.*

Ключові слова: *ХОП, ПХБ, ПАВ, дисперсно-фазовий розподіл, коефіцієнт гідрофобності, ХСК, БСК.*