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The octanol–air partition coefficient, K_{OA} , as a predictor of gas–particle partitioning of polycyclic aromatic hydrocarbons and polychlorinated biphenyls at industrial and urban sites

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Abstract: The main objectives of the research were to estimate the relationship between the gas–particle partition coefficient, K_p , and the octanol–air partition coefficient, K_{OA} , of polycyclic aromatic hydrocarbons, PAHs, and polychlorinated biphenyls, PCBs, at industrial and urban sites in the Vojvodina region, to compare the obtained slopes and intercepts of the $\log K_p$ vs. $\log K_{OA}$ relations with the results of regression analyses reported in previous studies and to assess the consistency between the particle-bound fractions predicted by the K_{OA} absorption model and the results obtained within field measurements. Fairly good $\log K_p$ – $\log K_{OA}$ correlations, with an average value of the correlation coefficients of 0.70, indicate that the partition coefficient K_{OA} can be used as a prediction parameter of the gas–particle partitioning processes for both classes of compounds. The results of modelling the atmospheric distribution of PAHs using the K_{OA} absorption model showed inconsistencies between the measured and predicted values of the particle-bound fraction, ϕ , of 1–2 orders of magnitude, while significantly higher discrepancies for PAHs in the Nap–Ace range were found. A similar variability of the measured/modelled ϕ values was obtained using the Junge–Pankow adsorption model, indicating the presence of particles enriched with PAHs. The conducted research showed that the K_{OA} -based approach was less suitable for predicting the gas–particle partitioning of PCBs in urban and industrial sites, compared to the Junge–Pankow model.

Keywords: gas–particle partitioning; polycyclic aromatic hydrocarbons; polychlorinated biphenyls; octanol–air partition coefficient.

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INTRODUCTION

Polycyclic aromatic hydrocarbons (PAHs) are formed during the processes of incomplete combustion of organic matter exposed to a temperature of 700 °C. The most frequent sources of PAHs include motor vehicles, re-suspended soils, oil- or gas-fired residential heaters, residential fireplaces, refineries, power plants and the food industry.^{1–3} PAHs are primarily emitted into the atmosphere and are mostly sorbed to particulate matter. However, PAHs are also present in the gaseous phase. PAHs having two or three rings (naphthalene, acenaphthene, anthracene, fluorene and phenanthrene) are present in the air, predominantly in the vapour phase. PAHs that have four rings (fluoranthene, pyrene, benz(*a*)anthracene, chrysene) exist both in the vapour and in the particulate phases, and PAHs having five or more rings (benz(*a*)pyrene, benzo(*g,h,i*)perylene) are found predominantly in the particulate phase.⁴ Due to their well-known carcinogenic, teratogenic and mutagenic properties, the Agency for toxic substances and disease registry has included 17 PAHs, with log K_{OA} (octanol–air partition coefficient) values in the range 5.13–11.01 in the list of toxic pollutants.

Polychlorinated biphenyls (PCBs) are dominantly synthetic organochlorines, widely manufactured in the mid 1900s for industrial use and commercially available until the late 1970s.⁵ The term PCBs refers to 209 congeners. The number and location of the chlorines in each congener (especially dioxin-like) govern both the environmental fate and toxicity. PCBs are extremely hydrophobic (log K_{OW} – octanol–water partition coefficient values from 4.34–7.12) and highly resistant to chemical reactions and biological degradation, which leads to their persistence, once they are emitted into the environment. The exposure to PCBs is reported to be a cause of cancer and impairment of the immune, reproductive, nervous and endocrine systems. Due to their health risk to the humans and to the environment, the usage of PCB is banned in numerous countries, according to the Stockholm Convention.

Their atmospheric distribution directly determines the fate, long-range transport (LRT) and transformation processes of semi-volatile organic compounds (SVOC), including PAHs, PCBs, polychlorinated dibenzo-dioxins and furans and organochlorine pesticides, in the atmosphere. Recent investigations have been focused on estimating, modelling and predicting the atmospheric partitioning of SVOC into the particle and vapour phases.^{1,6–12}

Several approaches for describing gas–particle partitioning of semi-volatile organic compounds have been proposed in the literature. The first model was developed by Junge and Pankow and it assumes that physical adsorption onto the aerosol surface is the main mechanism that governs the atmospheric distribution.^{13,14} The Junge–Pankow relation uses the sub-cooled liquid vapour pressure as the predictor of the particle bound fraction of SVOC. Another frequently used approach is the opposing Harner–Bidleman model, which assumes that absorp-

tion into the aerosol organic matter dominates the partition process.¹⁵ The absorption model proposes the octanol–air partitioning coefficient, K_{OA} , and the organic fraction of the aerosol, f_{OM} , as prediction parameters for the gas–particle partition coefficient.

The objectives of the study were to estimate the relationship between the gas–particle partition coefficient and octanol–air partition coefficient of PAHs and PCBs at industrial and urban sites in the Vojvodina region, and to compare the obtained slopes and intercepts of the $\log K_p$ vs. $\log K_{OA}$ relation to the results of regression analyses reported in the literature. An assessment of the consistency between the particle-bound fraction, ϕ , predicted by the K_{OA} absorption model and the ϕ obtained from field measurements was also one of the goals.

EXPERIMENTAL

Collection of air samples

The air sampling campaign was conducted during the APOPSBAL FP5 project, in the early summer period (median temperature was 19 °C), at six selected urban and industrial localities in the Vojvodina region of Serbia. The sampling spots were located in Novi Sad and Pančevo, as cities with significant industrial activities. Three samples were collected in the industrial zone within the Oil Refinery of Novi Sad (locality N1), three samples were taken in the residential zone of Novi Sad in the proximity and downwind to the oil refinery (locality N2) and three air samples were collected from the third, heavy traffic contaminated, urban sampling spot, in the city centre of Novi Sad (locality N3). Two sampling spots in Pančevo were located in the industrial area – the Oil Refinery of Pančevo (locality P1) and the Chemical Industry of Pančevo (P2). The city centre of Pančevo was chosen as the third, urban locality (P3). Four samples of ambient air were taken from the localities P1 and P3 and three air samples from the sampling spot P2.

Three high volume ambient air samplers were used (one GV2360 Thermoandersen TSP sampler and two samplers that were made of stainless steel boxes equipped with an 8×10 inch filter holder and a 9 cm-diameter polyurethane foam filter holder, 30 cm long). The average total air sampled was 1600 m³/24 h for the GV2360 Thermoandersen TSP sampler and 900 m³/24 h for the other two samplers. One glass fibre filter (Whatmann, fraction $d_{ae} < 50 \mu\text{m}$) and two polyurethane foam filters (Gumotex Břeclav, density: 0.03 g m⁻³) were used for each sampling period. Prior to the sampling campaign, the glass fibre filters were heated at 450 °C for 5 h and the polyurethane foam filters were Soxhlet extracted with 1:1 acetone/hexane (Merck SupraSolv) using a Foss Tecator Soxtec 1045 HT-2 apparatus for 4 h at 120 °C. The glass fibre and polyurethane foam filters were wrapped in aluminium foil and then placed in a zipped plastic bag. Common usage of both types of sampling medium enabled the simultaneous collection of the suspended particles and gaseous phase of pollutants. All the samples were taken over a period of 24 h.

Analysis of samples

The samples were analyzed using GC–ECD (HP 5890) supplied with a Quadrex fused silica column 5 % Ph for PCBs, while 16 US EPA polycyclic aromatic hydrocarbons were determined in samples using a GC–MS instrument (HP 6890 – HP 5972) supplied with a J & W Scientific fused silica column DB-5MS. Analytical details and Quality Assurance / Quality Control measures were published earlier.^{12,16} All analytical procedures were performed in the

laboratories of the Research Centre for Environmental Chemistry and Ecotoxicology (RECETOX), Masaryk University, Brno, Czech Republic.

The statistical analysis was performed using Statistica 8.0 (StatSoft, Inc. USA).

RESULTS AND DISCUSSION

The selected localities, the cities of Novi Sad and Pančevo, located in the Pannonian Plain of the Autonomous Province of Vojvodina in Serbia, were defined as hotspots by UNEP, as the most jeopardized cities during the conflict period in 1999.

The cities of Novi Sad and Pančevo have similar characteristics: developed industrial activity, the River Danube runs through both cities and both have oil refineries in the industrial zones that were heavily damaged by explosions and fires. The city of Pančevo has the Petrochemical Industry, which was partly destroyed during the 1999 war conflict.

Gas-particle partitioning

Semi-volatile organic compounds (SVOCs) are present in the gas phase and attached to particles. The experimental value of the particle-bound fraction, ϕ / %, of each compound (PAHs and PCBs) was determined using the following equation:

$$\phi = \frac{c_P}{c_G + c_P} = \frac{K_P TSP}{1 + K_P TSP} \quad (1)$$

where c_P is the concentration of the compound on particles in $\text{ng } \mu\text{g}^{-1}$ of particles, c_G is the concentration of the compound in the gas phase in ng m^{-3} of air, K_P is the gas-particle partition coefficient in $\text{m}^3 \mu\text{g}^{-1}$ and TSP is the concentration of the total suspended particles in the ambient air in $\mu\text{g aerosol m}^{-3}$ of air. The results are presented in Table I.

The lowest variability of the ϕ values was observed among the group of PAHs of high molecular mass, starting with chrysene. Benzo(*b*)fluoranthene, benzo(*k*)fluoranthene, benzo(*a*)pyrene, indeno(1,2,3-*cd*)pyrene, dibenz(*a,h*)anthracene and benzo(*ghi*)perylene were close to 100 % particle-bound.¹² The exception was the locality P1 (Oil Refinery of Pančevo), where the PAHs with a high molecular mass were 50 % and less particle-bound. The unforeseen atmospheric distribution obtained for the sampling spot at the Oil Refinery in Pančevo did not indicate, *a priori*, the low concentration of the total suspended particles in the ambient air. The high concentration levels of polycyclic aromatic hydrocarbons in the gaseous phase or sorbed to fine nano-particles, which could not be collected by glass fibre filters, were probably responsible for gas-particle partitioning of the higher PAHs at the locality P1.

In the atmosphere of the selected sampling points, the PCBs were generally found in the gaseous phase. In the group of compounds with a $\log K_{OA}$ value

between 5–8,¹⁷ the median ϕ values of the PCBs corresponded to the median ϕ values of the PAHs. The exception was the locality P3 (city centre of Pančevo), where the fractions of the PCB congeners 52 and 101 sorbed to particles (7.04 and 10.63 %, respectively) were significantly higher than those of the PAHs. For the compounds with $\log K_{OA}$ values higher than 8, elevated ϕ values were detected for the PAHs, in comparison to the PCBs. The results for the fraction ϕ obtained in the present study were significantly lower than the previously published values. While in earlier studies of urban, rural and adjacent coastal areas, the PCBs were associated with the atmospheric particles even up to 47 %, ^{8,18–20} the present analyses showed that the values of the fraction ϕ lay within the interval 0–22.5 % (Table I).

Table I. Median particle-bound fractions, ϕ / %, of PAHs and PCBs at all sampling sites (Nap – naphthalene, Acy – acenaphthylene, Ace – acenaphthene, Flo – fluorene, Phe – phenanthrene, Ant – anthracene, Flu – fluoranthene, Pyr – pyrene, B(a)A – benzo(a)anthracene, Chr – chrysene, B(b)F – benzo(b)fluoranthene, B(k)F – benzo(k)fluoranthene, B(a)P – benzo(a)pyrene, I(123cd)P – indeno(1,2,3cd)pyrene, D(ah)A – dibenzo(a,h)anthracene, B(ghi)P – benzo(ghi)perylene)

PAHs	N1	N2	N3	P1	P2	P3
Nap	2.315	5.890	3.365	0.939	1.754	1.576
Acy	10.714	10.870	1.724	2.778	0.000	0.000
Ace	2.804	5.660	5.714	8.771	10.811	4.952
Flo	0.993	1.818	1.439	0.062	0.390	0.829
Phe	0.395	0.631	0.789	0.153	0.094	0.435
Ant	1.245	1.237	2.264	0.000	0.304	0.639
Flu	4.762	3.807	2.921	1.150	0.852	3.430
Pyr	5.665	6.480	3.173	1.072	1.995	4.802
B(a)A	41.176	66.138	43.529	27.390	53.846	33.561
Chr	33.065	30.369	35.357	8.563	28.205	33.996
B(b)F	97.388	98.022	94.211	36.614	93.500	91.905
B(k)F	96.685	96.284	95.149	42.006	95.050	92.922
B(a)P	100.000	100.000	100.000	23.333	100.000	100.000
I(123cd)P	100.000	100.000	100.000	48.589	100.000	100.000
D(ah)A	100.000	100.000	100.000	100.000	100.000	100.000
B(ghi)P	100.000	100.000	100.000	49.560	100.000	100.000
PCB 28	0.00	0.00	0.00	0.00	1.54	0.00
PCB 52	5.45	0.72	1.66	0.54	1.31	7.04
PCB 101	0.00	0.00	0.00	1.00	1.64	10.63
PCB 118	0.00	0.00	0.00	0.00	0.00	0.00
PCB 153	2.63	2.33	0.00	1.29	1.45	7.74
PCB 138	5.00	2.00	0.00	1.54	1.59	5.72
PCB 180	12.50	7.69	0.00	3.89	2.78	22.50

Correlation $\log K_P$ vs. $\log K_{OA}$

Assuming that the absorption into an organic film that coats the particles is the main mechanism of the gas–particle partitioning of SVOCs, the following

equation can be used for the prediction of the atmospheric distribution at 298 K.^{15,21}

$$\log K_P = \log \frac{c_P}{TSPc_G} = m_{K_{OA}} \log K_{OA} + b_{K_{OA}} \quad (2)$$

For the state of equilibrium, the slope of the $\log K_P - \log K_{OA}$ correlation is expected to have a value of +1. The intercept of Eq. (2) depends on the organic fraction of the aerosol, which determines the absorption capacity of the aerosol.²²

The K_{OA} values used in Eq. (2) were cited or calculated using the equation:¹⁷

$$K_{OA} = \frac{K_{OW}RT}{H} \quad (3)$$

where K_{OW} is the octanol–water partition coefficient,¹⁷ T is the absolute temperature and H represents the constant in the Henry Law.¹⁷

The plots obtained as the result of linear regression analysis of the $\log K_P$ vs. $\log K_{OA}$ values for the PAHs at the six localities are shown in Supplementary Material, Fig. 1-S.

All the results were statistically significant, with the critical p -value less than 0.05. The slopes of Eq. (2) ranged from 0.43 to 0.56, with an overall average of 0.51, while the intercepts varied from -7.09 to -7.59 (average: -7.33). The values of the correlation coefficient (R^2) ranged between 0.60 and 0.78, with an average value of 0.70.

The resulting regression for PAHs is:

$$\log K_P = 0.51 \log K_{OA} - 7.33 \quad (4)$$

The regression plots of $\log K_P - \log K_{OA}$ for the PCBs are given in Supplementary material, Fig. 2-S.

For the statistically significant cases ($p < 0.05$), the slopes of the $\log K_P$ vs. $\log K_{OA}$ correlations ranged from 0.16 to 0.37 (average: 0.24). In addition, the intercepts of the plots were in the range from -5.25 to -7.52 , with an average value of -6.12 ($R^2 = 0.59-0.86$, average: 0.70). The results of the linear regression analysis of the $\log K_P$ vs. $\log K_{OA}$ plots indicated statistical insignificance for the localities: N3, P2 and P3 ($p > 0.05$). This might be due to the low concentration levels of PCBs in the particulate phase and the small number of individual congeners which were present in the particulate phase above the detection limit.

The resulting regression of the $\log K_P - \log K_{OA}$ correlation for PCBs is presented by Eq. (5):

$$\log K_P = 0.24 \log K_{OA} - 6.12 \quad (5)$$

The correlations obtained from the $\log K_P - \log K_{OA}$ plots in the present and earlier investigations are presented in Table II.

Table II. Correlations obtained from the $\log K_P$ vs. $\log K_{OA}$ plots in the present study and previously reported studies

Equation	Category of sampling site	Reference
PAHs		
$\log K_P = 0.51 \log K_{OA} - 7.33, R^2 = 0.70$	Urban and industrial	Present study
$\log K_P = 0.79 \log K_{OA} - 10.01, R^2 = 0.97$	From urban to rural	21
$\log K_P = 0.829 \log K_{OA} - 10.263, R^2 = 0.999$	Urban	15
$\log K_P = 0.83 \log K_{OA} - 9.89, R^2 = 0.87$	Heavy traffic urban	10
PCBs		
$\log K_P = 0.24 \log K_{OA} - 6.12, R^2 = 0.70$	Urban and industrial	Present study
$\log K_P = 0.55 \log K_{OA} - 8.20, R^2 = 0.79$	From urban to rural	21
$\log K_P = 0.654 \log K_{OA} - 9.183, R^2 = 0.876$	Urban	15
$\log K_P = 0.735 \log K_{OA} - 9.947, R^2 = 0.918$	Urban	23
$\log K_P = 0.54 \log K_{OA} - 8.23, R^2 = 0.82$	Urban	22
$\log K_P = 0.57 \log K_{OA} - 7, R^2 = 0.67-0.93$	Industrial	7

The quite good correlations between $\log K_P$ and $\log K_{OA}$, with an average value of the correlation coefficients of 0.70, indicate that the partition coefficient K_{OA} can be used as a prediction parameter of the gas-particle partitioning processes for both classes of compounds. The steeper slopes and higher intercepts of the linear regression analyses for the PAHs and PCBs obtained in previous studies at urban, rural, industrial and heavy traffic contaminated zones^{7,10,15,21-23} indicate to states closer to equilibrium, contrary to the present results (Table II). In addition to non-equilibrium in the atmospheric heterogeneous solid-gas system, the presence of several other phenomena, *e.g.*, variability among the activity coefficients in the organic matter, γ_{OM} , and in the surrogate of organic matter, octanol, γ_{oct} and adsorption of chemicals onto the surface of the particles, could result in the slopes differing from the theoretical value of +1.^{10,24}

The K_{OA} absorption model

Assuming that the entire organic matter of the aerosol is available to absorb gaseous compounds, the K_{OA} absorption model, given by Eq. (6), can be used to predict the values of partition coefficient K_P , knowing the coefficient K_{OA} and the organic fraction of the aerosol, f_{OM} :¹⁵

$$\log K_P = \log K_{OA} + \log f_{OM} - 11.91 \quad (6)$$

The values of the particle-bound fraction, ϕ , can be calculated using the partition coefficient, K_P , and the concentration of suspended particles in the ambient air, TSP , by applying Eq. (7):

$$\phi = \frac{K_P TSP}{1 + K_P TSP} \quad (7)$$

The modelled and measured particle-bound fractions were compared in order to estimate the validity of the K_{OA} absorption model. The fraction of the organic matter in the atmospheric particles was assumed to be $f_{OM} = 20\%$, which is the value expected for urban aerosols.¹⁵

The ratios between the measured ϕ values and the ϕ predicted using the K_{OA} model ($\log \phi_{\text{measured}}/\phi_{\text{predicted}}$) for PAHs are presented in Fig. 1. The experimental results for the PAHs of higher molecular mass (B(b)F, B(k)F, B(a)P, I(123cd)P, D(ah)A and B(ghi)P) were in line with the modelled fractions. The gap between the estimated and measured ϕ values was less than one order of magnitude for the medium molecular mass PAHs: phenanthrene, fluoranthene, pyrene and benz(a)anthracene. Chrysene was barely over predicted. An underestimation in the range of one to two orders of magnitude was observed for the low molecular mass PAHs (fluorene and anthracene), with a higher disagreement for acenaphthylene and acenaphthene (two orders of magnitude), and for naphthalene (even three orders of magnitude). The highest variability of the ϕ value was registered for anthracene, which indicated to different emission sources at the measuring points.

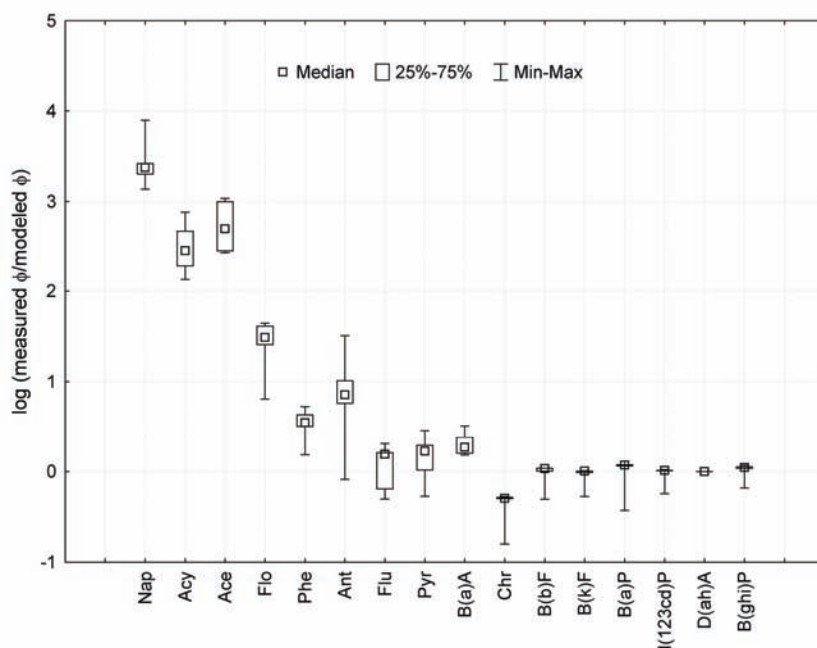


Fig. 1. Ratios of the modelled (K_{OA} absorption model) and measured particle-bound fraction (logarithmic) for PAHs.

Previously reported results on the atmospheric distribution of PAHs distinguished an inconsistency between the measured and predicted ϕ values of 1–2

orders of magnitude,^{15,25} while a significantly higher discrepancy for PAHs in the range Nap–Ace was obtained in the present study. The differences could be explained by the presence of a non-exchangeable, inert fraction of the PAH compounds in the aerosols and a slow re-equilibrium process between the PAH molecules in the gaseous phase and freshly emitted PM in the urban and industrial environments. A similar variability of the measured/modelled ϕ values was obtained using the Junge–Pankow adsorption model,¹² once again indicating to the existence of particles enriched with PAHs, whereby the main mechanism which governed the gas–particle partitioning of the PAHs remains unknown.

The median values and variability of the measured/modelled ϕ values for the PCB congeners are presented in Fig. 2.

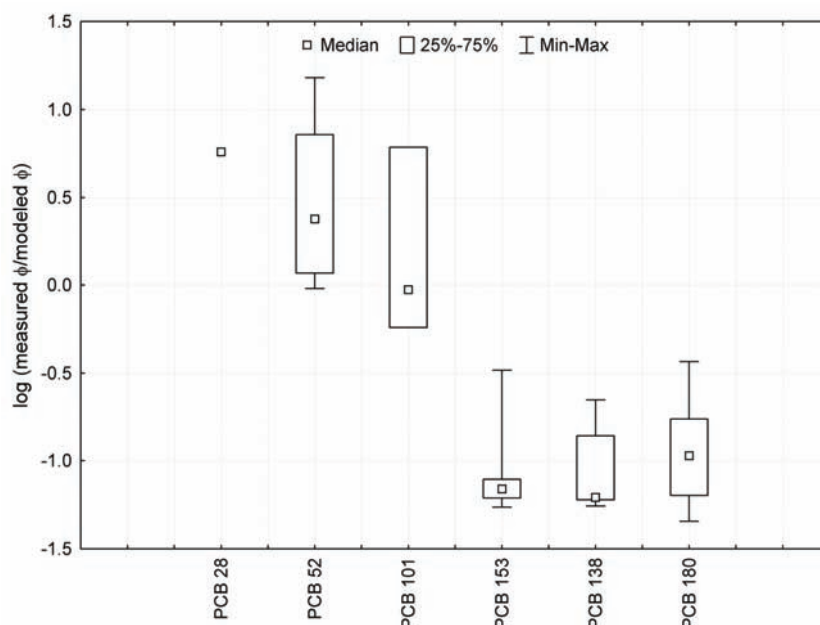


Fig. 2. Ratios of the modelled (K_{OA} absorption model) and measured particle-bound fraction (logarithmic) for PCBs.

The median values of the measured and modelled particle-bound fraction of the PCB congener 101 were in line. The congeners PCB 28 and 52 were underestimated by less than one order of magnitude, while the heavier PCB congeners (PCB 138, PCB 153 and PCB 180) were over predicted (by up to one order of magnitude).

These results are in good agreement with the results of previously published studies on the modelling of the atmospheric distribution of PCB congeners.⁹ The investigation showed that the K_{OA} -based approach was less suitable for the gas–

–particle partitioning of PCBs in urban and industrial sites, compared to the Junge–Pankow model.¹² The same observation was obtained in previously reported studies of urban²² and rural⁹ localities, while the results of Harner and Bidleman at urban sampling sites lead to the opposite conclusion.¹⁵

CONCLUSIONS

The present research was conducted in two industrial cities, Novi Sad and Pančevo, in the Province of Vojvodina, Serbia, with similar geoecological and industrial characteristics, defined as the hotspots in Serbia by UNEP.

The particle-bound fractions of the PAHs at the urban and industrial localities ranged from less than 1 to 100 %, which is in agreement with previously reported values. The PCB congeners (28, 52, 101, 118, 138, 153, and 180) were generally found in a gaseous phase in the atmosphere of the sampling sites. The results for the fraction ϕ were significantly lower than previously published values. While the studies in different countries (Korea, Turkey, and Greece) in urban, rural and adjacent coastal areas indicated that PCBs were sorbed on particles even up to 47 %, the present analysis showed that the values of the fraction ϕ lay within the interval 0–22.5 %.

The quite good $\log K_P - \log K_{OA}$ correlations, with an average value of the correlation coefficient of 0.70 for PAHs and PCBs, indicated that the partition coefficient K_{OA} could be used as a prediction parameter of the gas–particle partitioning processes for both classes of compounds. The obtained lower values for the slopes could indicate to a slow re-equilibrium between PAHs and PCBs in a gaseous phase and freshly emitted particulate matter in the urban and industrial environment, variability among the γ_{OM} and γ_{oct} , and adsorption of chemicals onto the surface of the particles.

Previously reported studies on the modelling of the atmospheric distribution of PAHs using the K_{OA} absorption model indicated inconsistency between the measured and predicted ϕ values by 1–2 orders of magnitude, while the present study showed a significantly higher discrepancy for PAHs in the range Nap–Ace. The results of this could be explained by the presence of a non-exchangeable, inert fraction of PAH compounds in the suspended particles. A similar variability of the measured/modelled ϕ values was obtained using the Junge–Pankow adsorption model, indicating to the presence of PAHs enriched particles. The research showed that the K_{OA} -based approach was less suitable for gas–particle partitioning of PCBs in urban and industrial sites, compared to the Junge–Pankow model.

The analysis of the residues of PAHs and PCBs in the ambient air was performed for the first time in the Vojvodina region, in order to obtain non-existing data for gas–particle partitioning processes at industrial and urban sites in this part of the western Balkan Region.

SUPPLEMENTARY MATERIAL

The plots of linear regression analysis of the $\log K_p$ vs. $\log K_{OA}$ values for the PAHs at the six localities and the regression plots of $\log K_p - \log K_{OA}$ for the PCBs are available electronically from <http://www.shd.org.rs/JSCS/>, or from the corresponding author on request.

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ИЗВОД

КОЕФИЦИЈЕНТ РАСПОДЕЛЕ K_{OA} КАО ПРЕДИКТОР АТМОСФЕРСКЕ ДИСТРИБУЦИЈЕ ПОЛИЦИКЛИЧНИХ АРОМАТИЧНИХ УГЉОВОДНИКА И ПОЛИХЛОРОВАНИХ БИФЕНИЛА НА ИНДУСТРИЈСКИМ И УРБАНИМ ЛОКАЛИТЕТИМА

ЈЕЛЕНА РАДОНИЋ, МИРЈАНА ВОЈИНОВИЋ МИЛОРАДОВ, МАЈА ТУРК СЕКУЛИЋ,
ЈЕЛЕНА КИУРСКИ, МАЈА ЂОГО и ДУШАН МИЛОВАНОВИЋ

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Рад приказује зависност коефицијената расподеле РАН и РСВ између гасовите и чврсте суспендоване фазе у атмосфери индустријских и урбаних локалитета региона Војводине од коефицијената K_{OA} , поређење добијених нагиба и одсечака корелације $\log K_p - \log K_{OA}$ са резултатима регресионе анализе из претходних истраживања и одступање удела РАН и РСВ у суспендованим атмосферским честицама од вредности процењених коришћењем апсорпционог K_{OA} модела атмосферске дистрибуције. Задовољавајућа корелација $\log K_p - \log K_{OA}$, са просечном вредношћу коефицијента корелације 0,7, указује да се коефицијент K_{OA} може користити за предвиђање партиције између гасовите и чврсте суспендоване фазе у атмосфери, за обе класе једињења. Претходним истраживањима предикције атмосферске дистрибуције РАН употребом апсорпционог K_{OA} модела добијена су одступања измерених од моделованих вредности ϕ за 1–2 реда величине, док мерења спроведена у оквиру истраживања указују на значајно већу неусаглашеност за нафтален, аценафтилен и аценафтен. Слични резултати одступања измерених и моделованих ϕ вредности добијени су и применом адсорпционог Junge–Pankow модела, што недвосмислено указује на присуство атмосферских честица са високим садржајем РАН на одабраним мерним местима. Истраживање је показало да се боља процена партиције РСВ на урбаним и индустријским локалитетима добија коришћењем Junge–Pankow модела, у односу на апсорпциони модел базиран на коефицијенту расподеле октанол–ваздух.

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