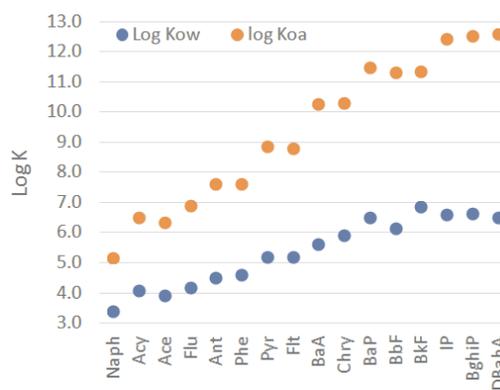
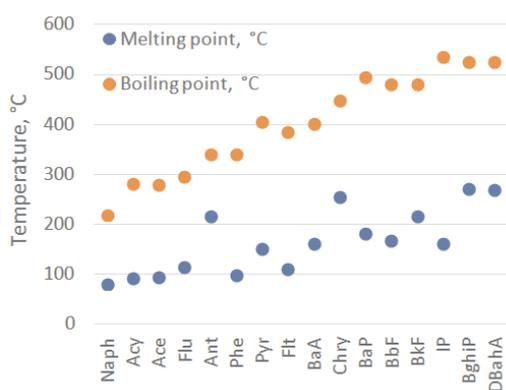


# Assessment of PAH pollution levels, key sources and trends: contribution to analysis of the effectiveness of the POPs Protocol

## Progress Report



Technical Report 2/2020



**MSC-E Technical Report 2/2020**

**June 2020**

**Assessment of PAH pollution levels, key sources  
and trends: contribution to analysis of the  
effectiveness of the POPs Protocol**

**PROGRESS REPORT**

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## SUMMARY

This progress report provides preliminary outcome of MSC-E activities performed in accordance with the bi-annual workplan of the Convention for 2020-2021 [ECE/EB.AIR/144/Add.2]. In particular, a number of aspects related to the contemporary pollution levels of Polycyclic Aromatic Hydrocarbons (PAHs), their trends, and population exposure are discussed in the report. This work can be considered as the contribution to the activities of TFTEI and TFH, aimed at the analysis of the effectiveness of the POPs Protocol with regard to the reduction of unintentional releases of PAHs.

PAHs comprise a large group of semi-volatile, hydrophobic organic compounds ubiquitous in the environment. Many of PAHs are known or suspected to have carcinogenic, mutagenic, and teratogenic properties that pose risk to human health and ecosystems. High levels and lack of decrease of PAH air concentrations in the EMEP countries during two recent decades have been indicated as an important issue in the Long-term Strategy of the Convention [ECE/EB.AIR/2018/1/Rev.1]. The Strategy highlights importance of continued scientific research that can support additional efforts for the reduction of unintentional releases of PAHs in the EMEP region and especially for countries of Eastern Europe, the Caucasus and Central Asia.

Taking into account long-range atmospheric transport, accumulation in the environment, and adverse effects on human health, PAHs are considered as priority pollutants in the regulatory activities of many international (WHO, HELCOM, AMAP, OSPAR, EU, etc.) and national (USA, Canada, China, etc.) organizations. Particular attention is paid to the compilation of inventories of PAH emissions, monitoring of air pollution levels, content in various products, and exceedances of guideline values as well as the assessment of population exposure and harmful effects. Within EU a new POPs Regulation (EU) 2019/1021<sup>1</sup> has been recently adopted that contains specific control measures for POPs (including PAHs) aimed at protecting human health and the environment.

Many of PAHs are considered to be hazardous to human health and environment due to their carcinogenic, mutagenic, and teratogenic properties, liver and kidney toxicity, hematological effects, pulmonary and respiratory effects, neurotoxicity. In addition, some of the PAHs are classified as very toxic for aquatic environment in accordance to the EU CLP Regulation<sup>2</sup>. Furthermore, chemical transformations of PAHs in the atmosphere can lead to the formation of other groups of toxic pollutants, such as nitrated and oxygenated PAHs, which may induce more significant toxic effects than their parental PAHs.

Approaches to the assessment of PAH pollution levels and adverse effects are often based on the use of B(a)P as a marker compound. However, it should be noted that air quality standards for B(a)P concentrations are still not globally defined, and different limit values are established by various organizations and countries to perform assessment of exceedances. Besides, different methodologies and different number of PAHs are used for the evaluation of population exposure to mixture of toxic

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<sup>1</sup> Council Decision 2004/259/EC of 19 February 2004 concerning the conclusion, on behalf of the European Community, of the Protocol to the 1979 Convention on Long Range Transboundary Air Pollution on Persistent Organic Pollutants

<sup>2</sup> Regulation (EC) No 1272/2008 (CLP) of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006

PAHs. In particular, 4 PAHs are included in LRTAP POP Protocol, 8 PAHs in the EU REACH Regulation, and US EPA Priority list contains 16 PAHs. The use of extended list of PAHs may help to estimate exposure of population to mixture of toxic PAHs more accurately.

PAHs are mostly released to the environment as unintentional by-products of incomplete combustion of biomass and fossil fuels. Main categories of anthropogenic PAH emissions include domestic burning of wood and coal, industrial activities, road transport, and agricultural sources. It should be noted that the residential combustion sector is also among the most significant contributors to the PM emissions and aerosol particles, emitted from the combustion processes, may be enriched by the toxic PAH compounds.

Despite the application of a number of restrictive measures regarding PAHs in recent decades, long-term risks of PAH pollution still exist, and levels of unintentionally released PAHs remain a concern. Available monitoring data and model predictions show that PAH contamination levels in EMEP countries have not changed significantly over the past twenty years. High level of annual mean B(a)P air concentrations, exceeding the EU target value, is still characteristic of some of the countries of Central Europe as well as of some of the EECCA countries. Furthermore, significant part of the population of EMEP countries lives in areas with exceeded the WHO reference B(a)P air concentration level.

Along with the analysis of long-term changes in PAH pollution levels and exceedances of air quality guidelines, the report provides an overview of information on physical-chemical properties of toxic PAHs, reported national inventories and expert estimates of PAH emissions as well as of the approaches to assess population exposure to PAH pollution. In addition, importance of consideration of wider list of toxic PAHs is emphasized and experimental model simulations are carried out to estimate population exposure to mixture of 16 toxic PAHs. Particular attention is also given to the interaction of PAHs and PM in the atmosphere, and contribution of toxic PAHs to the adverse effects of aerosol particles. At further stages of this work specific attention will be given to the analysis of statistical significance of temporal trends. Besides, model estimates of source-receptor relationships will also be taken into account in the analysis of temporal changes. In particular, contributions national and foreign emissions as well as emission sectors to PAH pollution levels will be evaluated.

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## INTRODUCTION

This technical report presents the progress in the MSC-E work related to the analysis of PAH pollution levels in the EMEP countries, carried out in accordance with the bi-annual workplan of the Convention for 2020-2021 [ECE/EB.AIR/144/Add.2]. The report consists of six chapters. In Chapter 1 an overview of ongoing international and national regulatory activities on PAHs is provided. A summary of information on physical-chemical properties and behaviour of PAHs in the environment is given in Chapter 2. Information on toxicological properties of PAHs and approaches for the assessment of the toxicity of PAH mixtures is presented in Chapter 3. Inventories of PAH emissions to the atmosphere in the EMEP region and on the global scale are described in Chapter 4. Long-term changes of PAH pollution levels on the example of B(a)P are characterized in Chapter 5. Evaluation of population exposure to PAHs and exceedances of B(a)P air quality guidelines are discussed in Chapter 6. The Annex to the report provides a compilation of information on physical-chemical properties of 16 PAHs required for model assessment of PAH pollution levels.

### 1. INTERNATIONAL AND NATIONAL REGULATORY ACTIVITIES ON PAHs

Polycyclic aromatic hydrocarbons (PAHs) comprise a large group of semi-volatile, hydrophobic organic compounds ubiquitous in the environment. Many of PAHs are known or suspected to have carcinogenic, mutagenic, and teratogenic properties. Taking into account long-range atmospheric transport, accumulation in the environment, and adverse effects on human health, PAHs are considered as priority pollutants in the regulatory activities of many international and national organizations (WHO, HELCOM, AMAP, OSPAR, etc.). At the same time, there are no globally defined environmental standards for PAHs. In this section brief overview of various current regional and national regulations on PAHs, focusing on air quality objectives, is presented.

#### 1.1. The POPs Protocol under the UN ECE LRTAP Convention

Under the Convention on Long-range Transboundary Air Pollution (CLRTAP), the Protocol on POPs (in the Article 3.5) requires the Parties to reduce total annual emissions of PAHs from the level of the emission in the reference year by taking appropriate effective measures. The list of PAHs considered in the Protocol includes 4 compounds, namely, benzo(a)pyrene (B(a)P), benzo(b)fluoranthene (B(b)F), benzo(k)fluoranthene(B(k)F), and indeno(1,2,3-cd)pyrene (IP) (Annex III) .

Developed measures and control options, recommended for the reduction of PAH emissions from industrial processes as well as residential combustion and wood preservation installations, are listed in the guidance document on best available techniques to control emissions of persistent organic pollutants from major stationary sources [ECE/EB.AIR/2009/14, 2009].

Besides, important activity regarding further development of measures to reduce PAH emissions is the preparation of the Code of good practice for wood-burning and small combustion installations carried out by TF TEI [ECE/EB.AIR/2019/5, 2019]. This document is aimed to provide recommendations on good practices and best available techniques for domestic wood heating installations.

## 1.2. World Health Organization

The World Health Organization (WHO) recognized PAHs as carcinogenic air pollutants. To evaluate exposure and health effects of PAHs the methodology, applied by WHO, used B(a)P as a marker of PAH mixture. In particular, unit risk for lung cancer of carcinogenic fraction of PAHs was estimated to be  $8.7 \times 10^{-5}$  per  $\text{ng}/\text{m}^3$  of B(a)P [WHO, 2017]. In accordance with this approach, corresponding concentrations for lifetime exposure to B(a)P, producing excess lifetime cancer risks of 1/10 000, 1/100 000, and 1/1 000 000, were estimated to 1.2, 0.12, and 0.012  $\text{ng}/\text{m}^3$ , respectively. The reference level of 0.12  $\text{ng}/\text{m}^3$  for B(a)P was defined as a level of air concentrations that corresponded to excess lifetime cancer risk level of  $10^{-5}$ .

The WHO expert meeting on the future update of the WHO Air Quality Guidelines noted that along with carcinogenic effects, the evidence of non-cancer endpoints (e.g. cardiovascular system, neurodevelopment or effects on birth weight) was also recently recognized for B(a)P. Thus, taking into account non-cancer health effects as well as exceedances of EU target value 1  $\text{ng}/\text{m}^3$  in some European countries, health evidence for B(a)P and other toxic PAHs should be re-evaluated [WHO, 2016].

A number of recent WHO studies were devoted to investigation of the health risks from particular matter (PM) in correlation with chemical composition of PM [WHO, 2013a; WHO, 2013b]. Currently used WHO air quality guideline values for PM are set without taking into account the presence of hazardous substances in their composition. However, the carcinogenic effects of PM, originated from combustion sources, could be related to the carcinogenicity of the compounds, presented in PM chemical composition (e.g. PAHs and their nitro- and oxy- derivatives) [WHO, 2016].

Along with evaluation of PAH toxicity of atmospheric concentrations, B(a)P is also used as an indicator for estimation of PAH toxicity for drinking water. Based on carcinogenic properties of B(a)P, WHO sets out guideline value for B(a)P water concentrations equal to 0.7  $\mu\text{g}/\text{L}$ , which corresponds to lifetime cancer risk of  $10^{-5}$  [WHO, 2011].

## 1.3. International Agency for Research on Cancer

International Agency for Research on Cancer (IARC) evaluated the carcinogenic risk of PAHs to humans based on existing experimental data. About 60 PAHs were included in the IARC Monographs Programme [IARC, 2010]. Among the studied PAHs, benzo(a)pyrene, was classified as carcinogenic to humans (Group 1). Dibenzo(a,h)anthracene and benzo(a)anthracene were classified as probably carcinogenic to humans (Group 2A), while benzo(b)fluoranthene, benzo(j)fluoranthene, benzo(k)fluoranthene, chrysene, naphthalene and indeno(1,2,3-cd)pyrene were classified as possibly carcinogenic to humans (Group 2B). Other considered PAHs were evaluated to be not classifiable with regard to their carcinogenicity to humans (Group 3), because of limited or inadequate experimental evidence [IARC, 2010] (Table 1).

It was also mentioned that epidemiological studies on human exposure to individual PAHs were complicated by that these compounds never occurred in isolation in the environment rather being components of complex chemical mixtures [IARC, 2019].

**Table 1.** IARC classification of PAHs [IARC, 2010; IARC 2012]

PAH	Group	PAH	Group
Benzo(a)pyrene	1	Chrysene	2B
Benzo(a)anthracene	2A	Benzo(e)pyrene	3
Dibenzo(a,h)anthracene	2A	Fluoranthene	3
Benzo(b)fluoranthene	2B	Pyrene	3
Benzo(j)fluoranthene	2B	Fluorene	3
Benzo(k)fluoranthene	2B	Benzo(g,h,i)perylene	3
Indeno(1,2,3-cd)pyrene	2B	Anthracene	3
Naphthalene	2B	Phenanthrene	3

#### 1.4. The Stockholm Convention on POPs

PAHs are not currently listed among the POPs considered in the annexes of the Stockholm Convention. Nevertheless, a number of Parties (e.g. Germany, Poland) to the Convention includes PAHs in their national implementation plans (NIPs) as the substances of high concern, pointing out the need of monitoring of their content in environmental media. These NIPs are developed in accordance with the Article 7 of the Convention by each party and describe national obligations under this Convention. PAHs were proposed to be considered as new POP candidates to the Stockholm Convention by the World Wildlife Fund [WWF, 2005].

#### 1.5. EU Regulation

EU Commission proposed a Clean Air Programme for Europe which sets out new air quality objectives for the period up to 2030. The main regulative instrument for this purpose is Directive (EU) 2016/2284 on the reduction of national emissions of certain atmospheric pollutants which entered into force on 31 December 2016. PAHs are included in Tables A, C and D of Annex A of Directive (EU) 2016/2284. Member States shall prepare and update on a timely basis national emission inventories for PAHs, national emission projections for PAHs, and also draw up an informative inventory report.

The EU has established a target value for PAHs in air in the Directive 2004/107/EC. This value is defined in terms of concentration of B(a)P, which is used as a marker substance for PAHs. EU target value for B(a)P annual mean air concentrations was set to be equal 1 ng/m<sup>3</sup>. Similar threshold level of B(a)P air concentrations was also established as an air quality standard in a number of other countries in the EMEP domain (e.g. in the EECCA countries). Along with B(a)P, the Article 4 of the Directive 2004/107/EC requires that each Member State shall monitor other PAHs (benzo(a)anthracene, benzo(b)fluoranthene, benzo(j)fluoranthene, benzo(k)fluoranthene,

indeno(1,2,3-cd)pyrene, and dibenzo(a,h)anthracene) at the same monitoring sites to assess the contribution of benzo(a)pyrene in contamination of ambient air.

Some Member States have set their own environmental quality standards for B(a)P and PAHs which are not mandatory (Table 2).

**Table 2.** Non-mandatory ambient air quality standards for the B(a)P [Ravindra et al., 2008]

Country	Limit value <sup>3</sup> (ng/m <sup>3</sup> )	Guide value <sup>4</sup> (annual average) (ng/m <sup>3</sup> )
Belgium	1.0	0.5
Croatia	2.0	0.1
Germany	-	10.0
Netherlands	1.0	0.5
France	0.7	0.1
Italy	1.0	-
Sweden	-	0.1
UK	-	0.25

On 25 June 2019 new POPs Regulation (EU) 2019/1021 was published in the EU Official Journal [ECHA, 2019]. Under revised POPs Regulation, ECHA (European Chemicals Agency) has responsibility for administrative, technical and scientific aspects of the implementation of this Regulation and the exchange of information. One of the main new tasks of ECHA under new POPs Regulation is supporting identification of new POPs substances for listing in the Stockholm Convention and Protocol to the Convention on Long-Range Transboundary Air Pollution on Persistent Organic Pollutants.

ECHA takes into consideration 4 PAHs under POPs Regulation and 8 PAHs under REACH Regulation (see Table 3). All of these PAHs are classified as carcinogens of Category 1B and as very toxic for aquatic organisms [EC, 2008].

**Table 3.** Classification of 8 PAHs according to EU CLP Regulation.

Name	Carcinogenicity	Mutagenicity	Toxicity for reproduction	Aquatic acute toxicity	Aquatic chronic toxicity
Benzo(a)pyrene	Cat. 1B	Cat. 1B	Cat. 1B	Cat. 1	Cat. 1
Benzo(e)pyrene	Cat. 1B	-	-	Cat. 1	Cat. 1
Benzo(a)anthracene	Cat. 1B	-	-	Cat. 1	Cat. 1
Dibenzo(a,h)anthracene	Cat. 1B	-	-	Cat. 1	Cat. 1
Benzo(b)fluoranthene	Cat. 1B	-	-	Cat. 1	Cat. 1
Benzo(j)fluoranthene	Cat. 1B	-	-	Cat. 1	Cat. 1
Benzo(k)fluoranthene	Cat. 1B	-	-	Cat. 1	Cat. 1
Chrysene	Cat. 1B	-	-	Cat. 1	Cat. 1

<sup>3</sup> Limit value may not be exceeded

<sup>4</sup> Exceeding the guide value should be avoided

The REACH regulation (Entry 50 of Annex XVII) [EC, 2006] provided restrictions on the content of PAHs in various products (e.g. B(a)P content in car tyres or their parts should be below 1 mg/kg (0.0001 % by weight) and content of the sum of all listed PAHs below 10 mg/kg (0.001 % by weight)).

Commission Regulation (EU) No 835/2011 [EU, 2011] sets out limit values for B(a)P and the sum of benzo(a)pyrene, benzo(a)anthracene, benzo(b)fluoranthene, and chrysene in food stuff [HBM4EU, 2018].

The European Commission adopted a proposal for a revised drinking water directive [EU, 2017]. Parametric values for PAHs and B(a)P are included in Part B of the Annex I of the proposal for drinking water directive. This document sets out limit value for B(a)P, which is equal to 0.010 µg/L, and for the sum of considered PAHs (benzo(b)fluoranthene, benzo(k)fluoranthene, benzo(g,h,i)perylene, and indeno(1,2,3- cd)pyrene), which is equal to 0.10 µg/L.

## 1.6. HELCOM

PAHs are listed among the hazardous substances selected within the Helsinki Commission (HELCOM) for the integrated assessment of Baltic Sea pollution. For integrated assessment of the Baltic Sea contamination status uses core indicators, for which quantitative threshold values are set up. The core indicators provide the information on the selected substances of high concern to the Baltic Sea in accordance with the HELCOM Baltic Sea Action Plan and HELCOM monitoring programme. In particular, this list includes hazardous substances (or substance groups) are persistent, toxic and accumulate in biota and poses hazard to environment [HELCOM, 2013].

The following PAHs were selected for the monitoring and assessment benzo(a)pyrene, fluoranthene and anthracene (Table 4). Integrated assessment includes monitoring of the concentration of three PAHs in biota and sediments and comparison to specific threshold values.

**Table 4.** HELCOM hazardous substances indicator details and threshold values [HELCOM, 2018a].

Substance	Assessment	Threshold
Benzo(a)pyrene	Biota (primary)	5 µg/kg wet weight crustaceans and molluscs (EQS*)
Fluoranthene	Biota (secondary)	30 µg/kg wet weight crustaceans and molluscs (EQS)
Anthracene	Sediment (secondary) (Normalized to 5% TOC)	24 µg/kg dw sediment (QS from EQS dossier)

\* - Environmental Quality Standard

In accordance with the HELCOM core indicator report, major sources of PAHs in the Baltic Sea are shipping activities and atmospheric deposition [HELCOM, 2018b].

## 1.7. OSPAR Convention

PAHs are included in the list of contaminants, which are of interest under the Convention for the Protection of the Marine Environment of the North-East Atlantic (OSPAR). In particular, they are added to the List of Chemicals for Priority Action (Part A) [OSPAR, 2013]. PAHs are among the substances, for which OSPAR continues monitoring of pollution levels and evaluation of necessity for additional measures, including filling the knowledge gaps. Since downward trends of PAHs are not observed in all OSPAR assessment areas, additional actions might be considered, which make it possible to move towards the cessation target. Besides, it is supposed that OSPAR will update the background document on PAHs which will present information on environmental and regulatory status [OSPAR, 2019].

## 1.8. Arctic Monitoring and Assessment Programme

The Arctic Monitoring and Assessment Programme (AMAP) is a Working Group of the Arctic Council. 16 PAHs (US EPA priority PAH) are in the focus of this program due to their hazard for environment and accumulation by Arctic fauna. PAH concentrations are estimated for all environmental media including atmosphere (air, snow), terrestrial compartment (soil, biota), freshwater (water, sediment, biota) and seawater (water, sediment, biota).

AMAP Assessment Report 2016 points out that the set of 16 PAHs is not sufficient for risk assessment. Nitro-, oxy-, and hydroxy-PAHs, as well as heterocyclic PAHs (thiophenes, azaarenes) can contribute to total toxicity of PAHs for ecosystems [AMAP, 2017].

## 1.9. PAH regulation in USA

PAHs are included into the lists of priority pollutants prepared by the US EPA and Agency for Toxic Substances and Disease Registry (ATSDR). ATSDR considers 17 PAHs (acenaphthene, acenaphthylene, anthracene, benzo(a)anthracene, benzo(a)pyrene, benzo(e)pyrene, benzo(b)fluoranthene, benzo(g,h,i)perylene, benzo(j)fluoranthene, benzo(k)fluoranthene, chrysene, dibenzo(a,h)anthracene, fluoranthene, fluorene, indeno(1,2,3-cd)pyrene, phenanthrene, pyrene). For these pollutants monitoring of their concentrations in air, water, and soil and regulation are required. Selection of the PAHs is based on information on their harmful properties, probability of exposure to these PAHs, and availability of the monitoring methods [ATSDR, 1995].

The US EPA priority list includes 16 PAHs (similar to ATSDR list except of benzo(j)fluoranthene). Despite the fact that in most countries this list is not prescribed by law, EPA priority PAH list is often used for the assessment of exposure to PAH mixtures and estimations of hazard for environment. The list of 16 EPA PAHs was issued in 1976, and recent studies suggest that this list should contain more compounds of this group [Andersson and Achten, 2015].

PAHs are listed as hazardous air pollutants to be regulated under the US Clean Air Act [US Code, 2018]. Emissions of hazardous air pollutants, including PAHs, are covered by the Section 112 of the

Clean Air Act. PAHs are considered in this regulation as Polycyclic Organic Matter (POM) which contain organic substances with at least two aromatic rings, and which have a boiling point greater than or equal to 100 °C [US Code, 2018]. Guidance for locating and estimating air emissions from sources of POM [EPA, 1998] recommends use the 16 PAHs-list to estimate emissions of POM.

US EPA pays great attention to combustion in residential wood stoves. In 2015 US EPA updated clean air standards for residential wood heaters. In accordance with these standards all woodstoves sold in the USA are required to have a label which indicates that woodstove was tested in EPA accredited laboratory and meets EPA standards [EPA, 2015].

In addition, EPA established water quality criteria (Clean Water Act, 33 USC 1251 et seq) which contain recommended national limits for PAHs. With regard to drinking water, the Maximum Contaminant Level (MCL)<sup>5</sup> of 0.002 mg/L for benzo(a)pyrene (as marker of PAHs) and zero content as the Maximum Contaminant Level Goal (MCLG)<sup>6</sup> is established by the Safe Drinking Water Act [EPA, 2009].

## 1.10. PAH regulation in Canada

In Canada, evaluation and regulation of PAH pollution levels in Canada is performed using the Canadian Environmental Protection Act [CEPA, 1994]. Selected PAHs, namely, benzo(a)pyrene, benzo(b)fluoranthene, benzo(j)fluoranthene, benzo(k)fluoranthene, and indeno(1,2,3-cd)pyrene, are considered as the most toxic under CEPA and are included in the list of priority substances for the assessment. Canada legislative acts established limit values for B(a)P in ambient air (Table 5).

**Table 5.** Canadian ambient air quality objectives for B(a)P

Jurisdiction	Limit values	Reference
Alberta Ambient Air Quality Objectives and Guidelines	Benzo(a)pyrene: 0.30 ng/m <sup>3</sup> (annual average concentration)	Government of Alberta, 2019
Ontario Ambient Air Quality Criteria	Benzo(a)pyrene as a surrogate of total PAHs Annual: 0.01 ng/m <sup>3</sup> 24-hour: 0.05 ng/m <sup>3</sup>	Government of Ontario, 2019

For regulation of B(a)P content in drinking water in Canada the maximum acceptable concentration (MAC) equal to 0.04 µg/L is established. Ontario Drinking Water Quality Standards<sup>7</sup> provides stricter value of MAC for B(a)P equal to 0.01 µg/L [Health Canada, 2016].

<sup>5</sup> The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to MCLGs as feasible using the best available treatment technology and taking cost into consideration. MCLs are enforceable standards [EPA, 2009].

<sup>6</sup> The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety and are non-enforceable public health goals [EPA, 2009].

<sup>7</sup> Ontario Regulation 169/03; Safe Drinking Water Act, 2002 (<https://www.ontario.ca/laws/regulation/030169>)

### 1.11. PAH regulation in China

Air pollution levels in China are regulated using the Ambient Air Quality Standards<sup>8</sup>. The limit values for air pollutants are set depending on the Class of the region. Specifically, Class 1 is applied to special regions and national parks, whereas Class 2 is applied to all other areas. A number of recent studies China scientists paid special attention to the investigation of adverse effects of PM considering chemical composition of particles (including PAH content) [Kong *et al.*, 2010; Li *et al.*, 2017; Zhao *et al.*, 2020]. So, Table 6 demonstrates limit values, established for B(a)P, PM<sub>2.5</sub>, and PM<sub>10</sub> by Chinese government.

**Table 6.** Ambient air quality standards in China.

Pollutant	Limit values, $\mu\text{g}/\text{m}^3$	
	Class 1	Class 2
Benzo(a)pyrene	0.001 (annual)	0.001 (annual)
	0.0025 (24 hours)	0.0025 (24 hours)
PM 2.5	15 (annual)	35 (annual)
	35 (24 hours)	75 (24 hours)
PM 10	40 (annual)	70 (annual)
	50 (24 hours)	150 (24 hours)

It should be noted, that air quality standard in China regulates only B(a)P without consideration of other PAHs. Nevertheless, the most of Chinese studies of air pollution include 16 EPA PAHs for the risk assessment.

In summary, there is a lot of international and national regulations that are directed to reduction of PAH pollution levels as well as their content in the environment and in specific products. At the same time, different methodologies and different number of PAHs are used for the evaluation of population exposure to toxic PAHs by various international organizations and countries. For instance, 4 PAHs are included in POPs Protocol, 8 PAHs in REACH Regulation, and US EPA Priority list contains 16 PAHs. Selection of particular PAHs is based on carcinogenic and mutagenic properties.

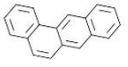
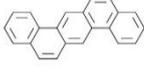
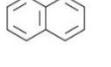
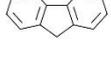
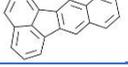
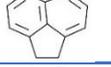
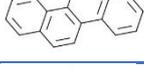
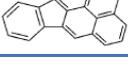
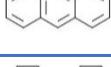
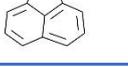
<sup>8</sup> National Standard GB 3095-2012 ([http://english.mee.gov.cn/Resources/standards/Air\\_Environment/quality\\_standard1/201605/W020160511506615956495.pdf](http://english.mee.gov.cn/Resources/standards/Air_Environment/quality_standard1/201605/W020160511506615956495.pdf))

## 2. PHYSICAL-CHEMICAL PROPERTIES OF PAHs AND DISTRIBUTION IN THE ENVIRONMENT

### 2.1. General characteristics

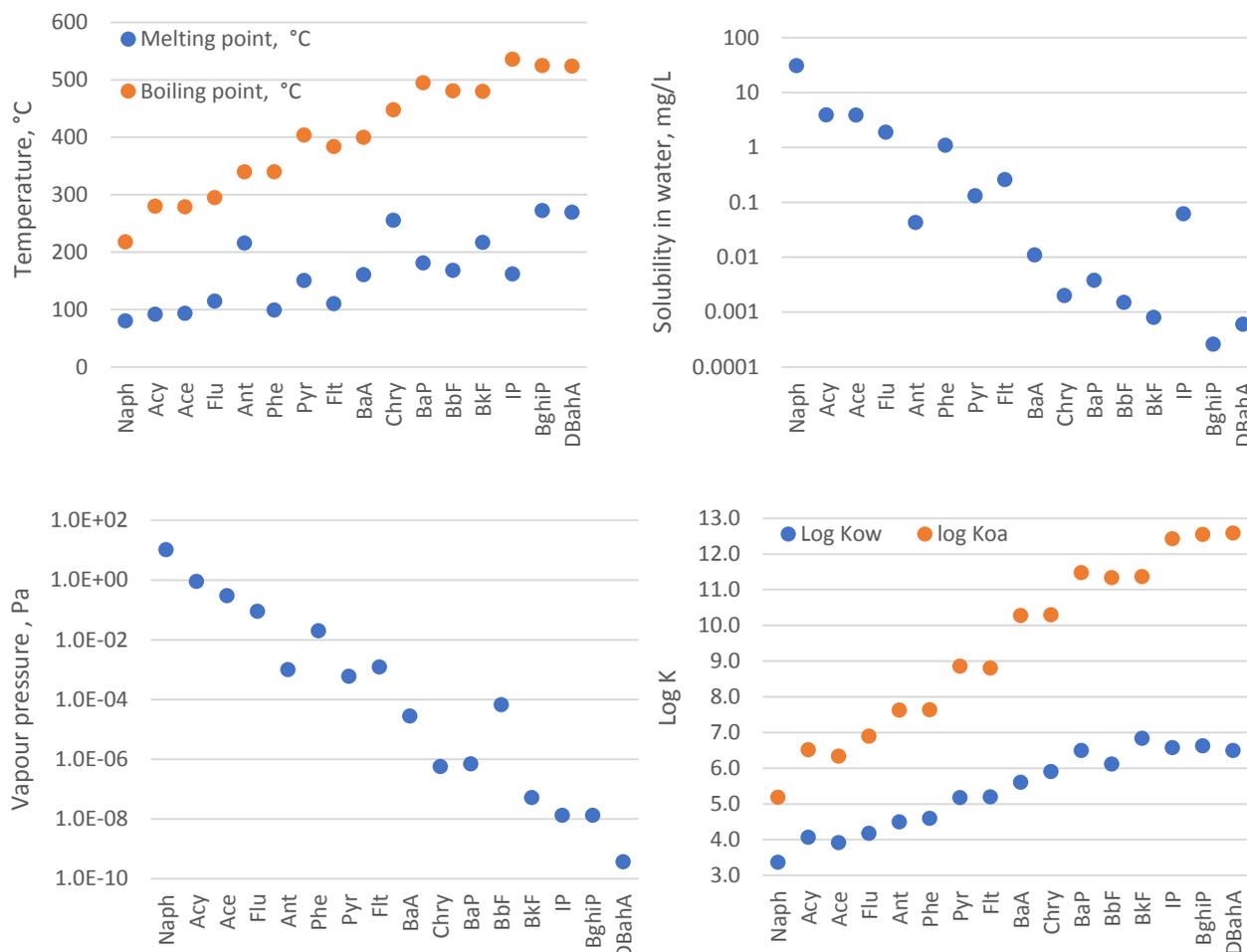
Polycyclic aromatic hydrocarbons include thousands of individual compounds but practically only 16 or less PAHs are usually determined as priority pollutants (Table 7). The considered PAHs can be divided into three groups: low-molecular weight PAHs, containing 2-3 aromatic rings, medium-molecular weight PAHs with 4 rings, and high-molecular weight PAHs (5 rings and more). These PAH groups are characterized by very different physical-chemical properties, which have impact on their long-range transport and partitioning between environmental compartments [Ma *et al.*, 2010]. Besides, some of the physical-chemical properties depend on temporal variability of environmental characteristics (e.g. temperature, humidity) that leads to significant seasonal variations of environmental fate of PAHs [Miura *et al.* 2019].

**Table 7.** Molecular structure of selected PAHs

Substance	Structure	M, g/mol	Substance	Structure	M, g/mol
Benzo(a)pyrene		252.31	Fluoranthene		202.26
Benzo(a)anthracene		228.29	Pyrene		202.25
Dibenzo(a,h)anthracene		278.36	Naphthalene		128.17
Benzo(b)fluoranthene		252.31	Fluorene		166.23
Benzo(k)fluoranthene		252.31	Acenaphthene		154.21
Chrysene		228.29	Benzo(g,h,i)perylene		276.33
Indeno(1,2,3-cd)pyrene		276.33	Anthracene		178.23
Acenaphthylene		152.19	Phenanthrene		178.23

PAHs are solid compounds with relatively high melting and boiling points that increase with increasing of molecular weight. At the same time, the values of vapor pressure and solubility in water of PAHs decrease with increasing molecular weight (Fig. 1) [WHO, 2010; Achten and Andersson, 2015]. As seen, the vapour pressure of individual PAHs differs by more than 10 orders of magnitude, which affects their predominant state and partitioning between the gaseous and particulate phases in the atmosphere. PAHs with two and three aromatic rings occur in atmosphere mainly in the gaseous phase, while PAHs with five rings and more are predominantly in the particulate phase. Besides, low-molecular weight PAHs are characterized by lower value of equilibrium partitioning coefficients between octanol and air ( $K_{OA}$ , Fig. 1) that also determine their presence in air

predominantly in the gaseous phase, as contrasted with high-molecular weight PAHs. Gas-particle partitioning strongly influences all the other processes (degradation and media exchange).



**Fig. 1.** Some physical-chemical parameters of considered PAHs (in the order of increasing of molecular weight)

Other important physical-chemical characteristics of PAHs include equilibrium partitioning coefficients between octanol and water ( $K_{OW}$ ), as well as between air and water ( $K_{aw}$ ). The octanol-water partition coefficient of PAHs is relatively high ( $\log K_{OW}$  value is from 3.37 to 6.84 [Lammel *et al.*, 2015]), so these compounds may be bio-concentrated in living organisms [ECHA, 2009], especially for PAHs with  $\log K_{OW}$  greater than 4.5 (See Table A.6 in the Annex A). The air-water partitioning coefficients of low- and high-molecular weight PAHs can differ by about 3 orders of magnitude ( $\log K_{aw}$  equal from -1.73 for naphthalene to -4.77 for benzo(g,h,i)perylene) that leads to a greater ability to wet deposition of PAHs with 5 rings or more compared to light PAHs [Ma *et al.*, 2010].

The behaviour of various PAH species in the environment is governed by several processes that include phase partitioning, exchange between, and degradation in the atmosphere and other environmental media. Brief description of these processes is given below, while more comprehensive review can be found in [Wang *et al.*, 2016; Keyte *et al.*, 2013; Ravindra *et al.*, 2008].

## 2.2. PAHs in ambient air

The most important processes that determine the fate of PAHs in the atmosphere are their partitioning between gaseous and particulate phases and chemical transformations (decomposition) [Lohmann and Lammel, 2004; Keyte et al., 2013]. As was mentioned, gas-particle partitioning of various PAHs depends on the amount of fused aromatic rings in their chemical structure. Other factors influencing these processes include variability of environmental conditions as well as the concentration and composition of aerosol particles (for instance, fraction of organic matter and black carbon in aerosol).

Recent studies showed that PAHs can be contained in condensable particles which are formed from hot gaseous phase during contact with cooler ambient air [Feng et al., 2018]. Herewith, among the different PAHs, compounds with 3 and 4 rings are assumed as the major part of condensable PM. In addition, a positive correlation is observed between the mass concentrations of PAHs contained in particles and concentrations of condensable PM [Li et al., 2017].

### *Degradation of PAHs*

Gas-phase PAHs have a short half-life in the atmosphere [Mackay et al., 2006]. Degradation of the gas-phase PAHs occurs predominantly by OH radical, while reactions with NO<sub>3</sub> radical and ozone are of minor importance [Mu et al., 2018]. Reaction with OH radical in most of the cases leads to a half-life in the air of less than one day [Vione et al., 2004]. For that reason, potential for long-range transport in the atmosphere is probably not high for PAHs in gaseous phase. However, when PAHs are included in the composition of aerosol particles, their lifetime in the atmosphere is expected to increase that leads to increasing of long-range transport potential [Blepp et al., 2012]. For particulate phase PAHs, degradation occurs mainly through the reactions with ozone.

It should be noted, that specificity of degradation processes affects seasonal variability of PAH fate in ambient air. The degradation rate depends on temperature and concentration of OH radicals which are higher in summer. Hence, concentrations of PAHs in air as well as long-range atmospheric potential are expected to be much higher in winter than in summer [Beyer et al., 2003, Lammel et al., 2009].

### *Transformation products of PAHs*

Chemical transformations of PAHs may result in formation of other group of toxic pollutants such as nitrated PAHs (nitro-PAHs) and oxygenated PAHs (oxy-PAHs). PAH derivatives are usually less volatile (in comparison with parent PAHs), respectively, they are more associated with particles [Vione et al., 2004].

Nitro-PAHs can be formed as a direct product of incomplete combustion, and also from nitration of PAHs in the atmosphere [WHO, 2003]. Chemical transformations can occur via gas phase reactions with OH and NO<sub>3</sub> radicals, or heterogeneous reactions on particles. Nitrated PAHs, are not well-

studied, but recently this group of the contaminants has received increasing attention due to their high toxicity [Nagato and Hayakawa, 2019]. Levels of nitro-PAH concentrations are lower comparing to the parent PAHs [Huang et al., 2014; Uno et al., 2017], however some studies showed their greater toxicity [Hasei et al., 2015; Gupta et al., 1996; Misaki et al., 2015; WHO, 2003].

Another group of contaminants which can be derived from parent PAHs is oxygenated PAHs (oxy-PAHs). Oxygenated PAHs can be formed along with other PAHs during incomplete combustion processes [Lundstedt et al., 2007]. Some oxy-PAHs are carcinogenic and mutagenic [Dasgupta et al., 2014; Idowu et al., 2019].

Despite availability of data on the toxicity of PAH derivatives, it is difficult to ensure systematic monitoring of their levels in ambient air. Main problem is a great variability of these substances, their low concentrations, and the need for highly sensitive analytical methods. In addition, their formation significantly depends on environmental conditions and concentrations of other contaminants, especially ozone, nitrogen oxides, and photooxidants [Lee, 2010]. Currently, model simulations of PAH derivatives is associated with high degree of uncertainty and is the subject of further research.

### 2.3. PAHs in water, sediments and soil

PAHs are widespread in all environmental media. As a rule, the half-life of PAHs in water, soil and sediments is significantly longer than in the atmosphere. Therefore, these media can accumulate significant amounts of PAHs. In addition, PAHs can undergo re-evaporation and gas exchange with water surfaces, soil and vegetation [Keyte et al., 2013]. Exchange between other environmental media also can occur.

The main source of PAHs in water is atmospheric deposition. It is estimated that up to 80% of PAHs enter water bodies through atmospheric deposition [Srogi, 2007]. Along with deposition to water surfaces, PAHs can enter water environment with surface runoff from the polluted areas. Other sources of PAHs in water include sewage treatment plants, diffuse sources, oil spillage and leakage, industrial effluents [Srogi, 2007; Manoli and Samara, 1999].

PAHs are relatively persistent in aquatic environments. Degradation of PAHs in surface water occurs due to direct sunlight photolysis. In the deep layers biodegradation processes are more important. Half-lives of considered PAHs in surface water and groundwater are presented in the Table 8.

Sediments can be regarded as important sink for PAHs, but exchange processes between sediments and water can also occur. These processes depend on the number of aromatic rings of considered PAHs. The sediments act as a secondary source of emissions for PAHs with three and four rings, while PAHs with five rings and more are deposited and accumulated in sediments [Cui et al., 2016].

Soil is another significant sink of atmospheric PAHs. Soil is regarded as a steady indicator of environmental pollution since low soil mobility of PAHs (log  $K_{oc}$  value is from 2.5 to 8.0). Soil may be possible source of PAHs pollution of groundwater. In addition, the contamination of soil can lead to accumulation of PAHs in vegetation and food chains [Mueller and Shann, 2006].

**Table 8.** Half-lives of PAHs in the environmental media [Mackay et al., 2006; ChemSpider database]

Substance	Surface water, hour	Groundwater, day	Sediments (estimated values), day	Soil, day
Benzo(a)pyrene	2-900	110 -1060	340	50-3180
Benzo(a)anthracene	3-1440	200-1400	540	50 - 6250
Dibenzo(a,h)anthracene	6-1440	720-1880	540	361-940
Benzo(b)fluoranthene	8.7-1440	720-1220	540	210-3285
Benzo(k)fluoranthene	3.8-1440	1770-4280	540	50-3180
Chrysene	4.4-1440	740-2000	540	50-1000
Indeno(1,2,3-cd)pyrene	900	>1000	340	75
Acenaphthylene	1020-1440	85-120	135	42-60
Fluoranthene	1440	280-880	540	40-2850
Pyrene	0.68-1440	420-3800	540	48-3100
Naphthalene	7-13200	1-258	340	2-770
Fluorene	768-1440	64-120	135	32-60
Acenaphthene	3-900	24-204	340	12-102
Benzo(g,h,i)perylene	1440-15600	1180-1300	540	50-3320
Anthracene	108-1440	100-920	540	3.3-2890
Phenanthrene	8.4-1440	32-400	540	2.5-2080

## 2.4. Basic physical-chemical characteristics of PAHs required for modelling

Physical-chemical properties are basic characteristics required for modelling of PAH fate in the environment. In order to predict long-range transport and distribution of different PAHs in the environment, multi-media modelling approach is usually applied. Model assessment of PAH pollution levels, presented in this report, is performed using the multi-media GLEMOS model (<http://en.msceast.org/index.php/j-stuff/glemos>). Key processes, covered in the model, include the transport, phase partitioning, degradation, exchange of PAHs between the atmosphere and other environmental compartments. The following main physical-chemical properties of PAHs are used in GLEMOS model:

- subcooled liquid vapour pressure ( $p_{OL}$ );
- octanol-water ( $K_{OW}$ ), octanol-air ( $K_{OA}$ ), organic carbon-water ( $K_{OC}$ ) partition coefficients;
- degradation rate constants for different environmental compartments;
- air-water Henry's law constant ( $K_H$ );
- washout ratio for the particulate ( $W_p$ ) and gaseous phase ( $W_g$ ).

Compilation of available data on the physical-chemical properties of 16 PAHs, used for parametrization of key processes, is included in Annex A. Among the considered PAHs, B(a)P is the most studied one with regard to the processes of gas-particle partitioning and degradation in the atmosphere. Taking this into account more complex model parameterizations of these processes are

currently applied for B(a)P comparing to other PAHs. In addition, there is ongoing activity on testing and application of newly developed process parameterizations in the GLEMOS model [Travnikov *et al.*, 2020].

It should be noted also, that parametrization of sorption of PAHs by organic and inorganic components of aerosol particles, as well as heterogeneous reactions of PAHs, are subject to considerable uncertainty [Shrivastava *et al.*, 2017]. For instance, degradation rate constants in air reported in literature may differ by 2-3 orders of magnitude. Other uncertainties concern temperature dependences of subcooled liquid-vapour pressure, coefficients of partitioning between different media (octanol-water, organic carbon-water, octanol-air), and degradation rates in other environment compartments.

### 3. TOXICITY AND HUMAN EXPOSURE TO PAHS

PAHs are highly hazardous for human health as well as for environment [Theakston, 2000]. Effects for human health include carcinogenicity and mutagenicity, reproductive toxicity, liver and kidney toxicity, hematological effects, pulmonary and respiratory effects, neurotoxicity, and skin irritation in case of direct contact [Danish EPA, 2013]. PAHs in ambient air may cause asthma [Karimi *et al.* 2015, Liu *et al.*, 2016]. Some PAHs are endocrine disrupters and may affect the immune system [WWF, 2005]. In addition, the presence of UV light may induce more toxic effects of PAHs, and their effects may be underestimated [MAFF, 2000].

#### 3.1. Routes of exposure

The main routes of exposure to PAHs for the general population include inhalation and ingestion [EFSA, 2008]. Some studies suppose that dermal contact also might have significant impact comparable with inhalation exposure [Strandberg *et al.*, 2018; Van Rooij *et al.*, 1993a,b].

The important route of human exposure to PAHs is through the lungs and respiratory tract after inhalation of aerosols and particles containing PAHs, due to the high carcinogenic potency of PAHs. Estimated intake of benzo(a)pyrene by inhalation route is about 20 ng/day per person (for general population) [EC, 2002].

Ingestion of PAHs can occur through food and drinking water. Contamination of food by PAHs may be due to presence of these substances in air, water, soil, and plants. The major source of PAHs for plants is atmospheric deposition [Knoche *et al.*, 1995; Wilcke, 2000]. Besides, plants can absorb PAHs through the root system from soil. Other important source of PAHs in the food may be specific processes which are used for cooking (especially heating, smoking, grilling and roasting processes). European Food Safety Authority estimated that the overall average dietary exposure in EU is ranged from 185 to 255 ng/day for benzo(a)pyrene, and from 1415 to 2136 ng/day for the sum of 8 PAHs. PAH intake from drinking-water is usually less significant comparing to the intake from food. However, these values could be equal, if water is contaminated by coal tar coatings of drinking-water distribution pipes [WHO, 2011].

Dermal exposure is possible during contact with contaminated soil or in cases of skin contact with materials containing PAHs. Among these materials soot, tar, petroleum products could be mentioned [EPA, 2017].

### 3.2. Toxicity and adverse effects

The main toxicological endpoints of PAHs include acute toxicity, short-term toxicity, carcinogenicity, mutagenicity, reproductive and developmental toxicity and other effects.

Studies on the acute toxicity of PAHs are limited. The LD50<sup>9</sup> values show that acute toxicities of PAHs are low to moderate [SCF, 2002a; ATSDR, 1995]. Among the 16 PAHs, only naphthalene is classified as harmful (if swallowed) in accordance with the EU CLP Regulation [ECHA, 2018].

A number of studies of the short-term effects have shown that PAHs can affect various tissues of experimental animals after oral administration. Some of the endpoints (e.g., for benzo(a)pyrene, acenaphthene, fluorantene, fluorene) are associated with effects on the liver, indicating varied degrees of hepatotoxicity. Other significant effects are related to immune response [Silkworth *et al.* 1995; SCF, 2002b; CCME, 2010]. In addition, exposure to benzo(a)pyrene may induce adverse hematologic effects in animals [Larsen, 2013; EPA, 2017].

The most of international and national regulations consider carcinogenic potential as the main reason for setting limit values for PAHs (see Section 1). Development of cancer can be associated with the route of exposure, for instance, ingestion causes tumors of the stomach, inhalation and direct instillation to respiratory tract led to lung tumors. However, this dependence is not always observed [IPCS, 1998].

Literature data demonstrate that the most of PAHs have evidence of mutagenicity/genotoxicity in vivo or in vitro (Table 9). For number of PAHs only in vitro data are available, so further investigations are required. Anthracene, naphthalene and pyrene have negative results in the most of (or in all) short term tests.

Reproductive and developmental toxicity of some of the PAHs (e.g. Benzo(a)pyrene and dibenzo(a,h)anthracene) was observed in several studies [IARC, 1983; EPA, 2017; SCF, 2002b]. It should be noted, that in most cases impact of B(a)P on reproduction and development is observed at relatively high doses in comparison with doses corresponded to carcinogenic effects.

Some PAHs have been identified as endocrine disrupting substances [Clemons *et al.*, 1998; Safe *et al.*, 1997]. Studies on the relationship between the effects of PAHs and the endpoints of endocrine toxicity are limited. The capability of PAHs to bind to endogenous receptors which act as the pathways of the endocrine response are the main evidence for the role of PAHs as endocrine disruptors [CCME, 2010].

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<sup>9</sup> Median lethal dose

The cardiovascular effects of PAHs consist in the potential for the development of atherosclerosis due to endothelial damage and changes in smooth muscle cells, which leads to their clonal expansion in the walls of arteries [SCF, 2002b].

**Table 9.** Evaluation of genotoxicity of considered 16 PAHs [SCF, 2002b]

Substance	Genotoxicity
Benzo(a)pyrene	Genotoxic
Benzo(a)anthracene	Genotoxic
Dibenzo(a,h)anthracene	Genotoxic
Benzo(b)fluoranthene	Genotoxic
Benzo(k)fluoranthene	Genotoxic
Chrysene	Genotoxic
Indeno(1,2,3-cd)pyrene	Genotoxic
Acenaphthylene	Inappropriate data
Fluoranthene	Limited evidence of genotoxicity
Pyrene	Not genotoxic
Naphthalene	Probably not genotoxic
Fluorene	Inappropriate data
Acenaphthene	Inappropriate data
Benzo(g,h,i)perylene	Genotoxic
Anthracene	Not genotoxic
Phenanthrene	Limited evidence of genotoxicity

### 3.3. Toxicity of PAH mixtures

Human health toxicity of a PAH mixture may be estimated through converting of the PAH concentrations in the mixture to an equivalent concentration of benzo(a)pyrene [EPA, 2010]. Historically, toxic equivalent factor (TEF) was calculated for 16 PAH, but recent studies include estimates for up to 88 PAHs both in gaseous and particle phases for more accurate estimation of carcinogenic potency of PAH mixtures [Samburova *et al.*, 2017]. For PAH derivatives (nitro-PAH, oxy-PAH) TEF also could be generated to estimate impact of these groups of contaminants [Wei *et al.*, 2015]. Total toxic equivalent concentration of PAH mixture can be calculated using the following equation:

$$TEQ_{total} = \sum c_n \cdot TEF_n, \quad (1)$$

where:  $TEQ_{total}$  - total toxic equivalent concentration of PAH mixture for assessment of carcinogenic potency;  $c_n$  - concentration of the individual PAH in the mixture;  $TEF_n$  - toxic equivalent factor for the individual PAH in the mixture (relative to the carcinogenic potency of B(a)P).

The TEF for B(a)P is defined equal to 1. The TEF values of the other PAHs represent a ratio of their toxicity to that of B(a)P. These TEFs can be applied to characterize the carcinogenic potency of each considered PAH and calculate B(a)P equivalent concentration of total PAH mixture (Table 10). This method does not take into account possible synergistic effects of PAH in mixtures, but it is significantly more cost-effective in comparison with testing in laboratories. The toxicity equivalent concentration is widely used to evaluate carcinogenic risk of PAH mixtures and may be applied for any environmental media.

**Table 10.** TEF for individual PAHs from literature

Substance	TEF [Samburova et al, 2017]	TEF [Bari, 2010]	TEF [Liu, 2009]
Benzo(a)pyrene	1	1	1
Benzo[e]pyrene	1	0.01	
Benzo(a)anthracene	0.1	0.1	0.005
Dibenzo(a,h)anthracene	5	1	1.1
Benzo(b)fluoranthene	0.1	0.1	0.1
Benzo(j)fluoranthene	0.1	0.1	
Benzo(k)fluoranthene	0.1	0.1	0.05
Chrysene	0.01	0.01	0.03
Indeno(1,2,3-cd)pyrene	0.1	0.1	0.1
Acenaphthylene	0.001	0.001	
Fluoranthene	0.001	0.001	0.05
Pyrene	0.001	0.001	0.001
Naphthalene	0.001	0.001	
Fluorene	0.001	0.001	
Acenaphthene	0.001	0.001	
Benzo(g,h,i)perylene	0.01	0.01	0.02
Anthracene	0.01	0.01	0.0005
Phenanthrene	0.001	0.001	0.0005

Similarly, the mutagenic equivalent concentration (MEQ) can be estimated for assessment of joint mutagenic potency of PAH mixtures.

$$MEQ_{total} = \sum c_n \cdot MEF_n, \quad (2)$$

where  $MEQ_{total}$  - total toxic equivalent concentration of PAH mixture for assessment of mutagenic potency;  $c_n$  - concentration of the individual PAH in the mixture;  $MEF_n$  - toxic equivalent factor for the individual PAH in the mixture (relative to the mutagenic potency of B(a)P).

Available estimates of MEF values for individual PAHs are listed in the Table 11 below.

**Table 11.** Estimates of MEF values for individual PAHs

Substance	MEF [Durant, 1996]
Benzo(a)pyrene	1
Benzo[e]pyrene	0.0017
Benzo(a)anthracene	0.082
Dibenzo(a,h)anthracene	0.29
Benzo(b)fluoranthene	0.25
Benzo(j)fluoranthene	0.26
Benzo(k)fluoranthene	0.11
Chrysene	0.017
Indeno(1,2,3-cd)pyrene	0.31
Acenaphthylene	5.6E-04
Benzo(g,h,i)perylene	0.19

### Assessment of the inhalation cancer risk of PAH mixtures

The inhalation cancer risk (ICR) from exposure of PAH mixtures can be estimated by using of formula [Bootdee et al., 2016; Jung et al., 2010; Jia et al., 2011; Sarkar and Khillare, 2012; Wiriya et al., 2013]:

$$ICR = TEQ \cdot IUR_{BaP} \quad (3)$$

$$Risk = ICR \cdot 10^6 \quad (4)$$

where *ICR* – inhalation cancer risk; *TEQ* - total toxic equivalent concentration of PAH mixture for assessment of carcinogenic potency; *IUR<sub>BaP</sub>* – the inhalation unit risk; *Risk* - societal inhalation cancer risk (number of cancer cases per million people). Values of *IUR<sub>BaP</sub>* , which can be used for assessment of inhalation cancer risk are listed in the Table 12:

**Table 12.** Estimates of the inhalation unit risk

	<i>IUR<sub>BaP</sub></i>	Reference
World Health Organization (WHO)	$8.7 \times 10^{-5} \text{ m}^3/\mu\text{g}$	WHO, 2000
Office of Environmental Health Hazard Assessment (OEHHA) of California Environmental Protection Agency (CEPA)	$1.1 \times 10^{-6} \text{ m}^3/\mu\text{g}$ for lifetime (70 years) PAH exposure.	Collins et al., 1998, OEHHA, 2003

Some studies use WHO and CEPA IUR values as upper and lower estimates of potential cancer risk [Sarkar and Khillare, 2012]. ICR value between  $10^{-6}$  and  $10^{-4}$  corresponds to medium cancer risk. If ICR value exceeds  $10^{-4}$  it may indicate high cancer risk [Bootdee et al., 2016].

Thus, many PAHs pose a serious risk to human health. At the same time, data for number of toxicological endpoints are limited and additional investigations are required. To assess the toxicity of PAH mixtures, approach of calculation of total toxic equivalent concentrations may be used. Besides, modelling results can be used to estimate the spatial and temporal distribution of indicators of the total population exposure, especially for urban areas.

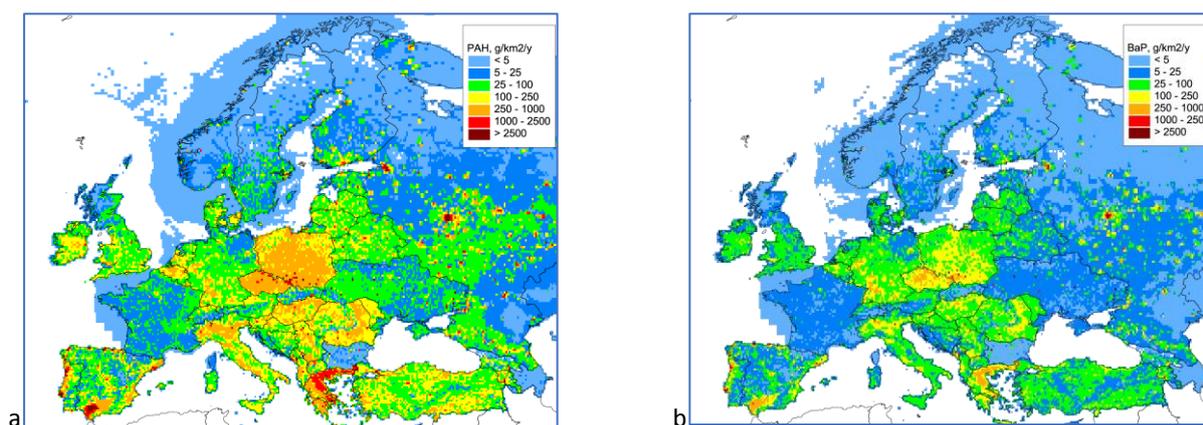
## 4. SOURCES OF PAH RELEASES TO THE ENVIRONMENT

Depending on the condition of formation, PAHs can be originated from pyrogenic or petrogenic sources [Manzetti, 2013]. Pyrogenic PAHs are mainly released to the atmosphere as unintentional by-products of incomplete combustion of biomass and fossil fuels [Keyte *et al.*, 2013]. Main categories of anthropogenic PAH emissions include domestic burning of wood and coal, industrial activities, road transport, and agricultural sources as well as forest fires and volcanic activities [Balmer *et al.*, 2019; Manzetti, 2013]. Petrogenic PAHs can be released to the atmosphere in course of oil production and refining processes, as well as a result of industrial spills and oil accidents [Ravindra *et al.*, 2008].

To monitor dynamics of unintentional releases of PAHs, official data on emissions are compiled within the EMEP region. Along with this a number of research-driven emission inventories are available for evaluation of temporal and spatial trends of PAH content in the environment as well as adverse effects.

### 4.1. PAH emissions within EMEP region

Regional scale inventories of sector-specific atmospheric emissions of selected 4 PAHs are being regularly produced by the EMEP countries [Tista *et al.*, 2018]. Compiled information for the EMEP region shows elevated levels of PAH emission fluxes ( $>0.25$  kg/km<sup>2</sup>/y) in the countries of Central and Southern Europe (e.g. Poland, the Czech Republic, Italy, Greece) (Fig. 2a). Besides, significant emission fluxes (0.025-0.25 kg/km<sup>2</sup>/y) are estimated for some of Western European and the EECCA counties (e.g. Russia, Ukraine). Lower levels of emissions ( $<0.025$  kg/km<sup>2</sup>/y) are reported for the countries of Northern Europe. In general, higher emissions are indicated for urban and densely populated areas.

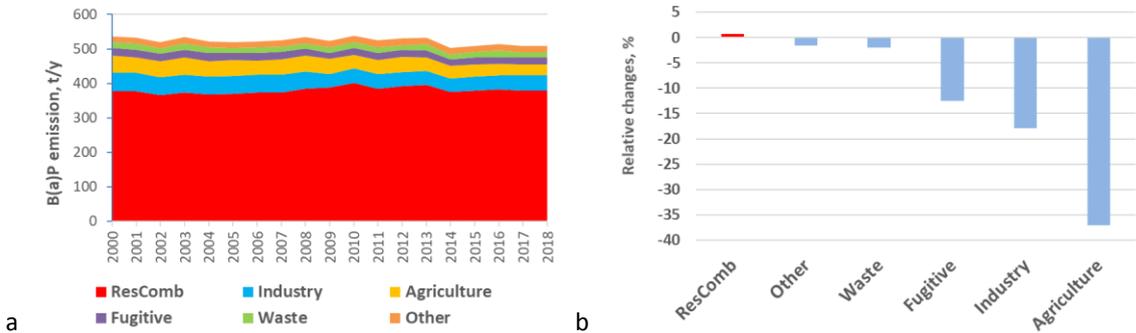


**Fig. 2.** Spatial distribution of 4 PAHs (a) and B(a)P (b) emissions in the EMEP region for 2017.

According to the reported emission data, average fractions of B(a)P, B(b)F, B(k)F, and IP in total 4PAH emissions are equal to 30%, 35%, 15%, and 20%, respectively. At the same time, for particular countries contributions of individual PAHs to the total national PAH emissions can be different. Along with this, spatial distribution of emissions of individual PAHs may differ. This, in particular, can be seen from the comparison of spatial distributions of 4 PAHs and B(a)P emissions in the EMEP countries shown in Fig.2a and b (e.g. for some of the countries in Central Europe).

Sector distribution of PAH emissions of the EMEP countries indicates the largest contribution (> 60%) to total emissions for the Residential combustion sector (Fig.3a). Following officially reported information, in the majority of countries dominating source of PAH emissions from this sector is wood combustion for domestic heating. At the same time, some of the countries are characterized by substantial contribution of coal combustion (e.g. Poland, Ireland). Along with the Residential combustion, significant emissions of PAHs are reported for industrial (~10%) and agricultural (~10-15%) activities.

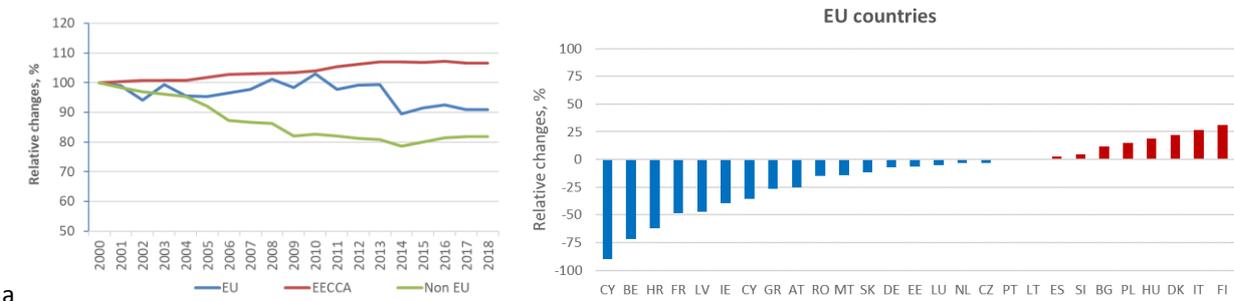
Time-series of total emissions of 4 PAHs in the EMEP region demonstrate almost the same emission level during the two recent decades. As an example, temporal changes of sector-specific B(a)P emissions during the period 2000-2018 are shown in Fig. 3.



**Fig. 3.** Long-term changes of sector-specific B(a)P emissions in the EMEP countries (a) and changes in % (b) from 2000 to 2018.

It is seen that B(a)P emissions from the Residential combustion sector did not change since 2000 (0.6%). At the same time, emissions from the other sectors tend to decrease with the largest changes for Agriculture and Industry sectors (-36% and -17%, respectively). However, these changes did not have significant effect on total emissions.

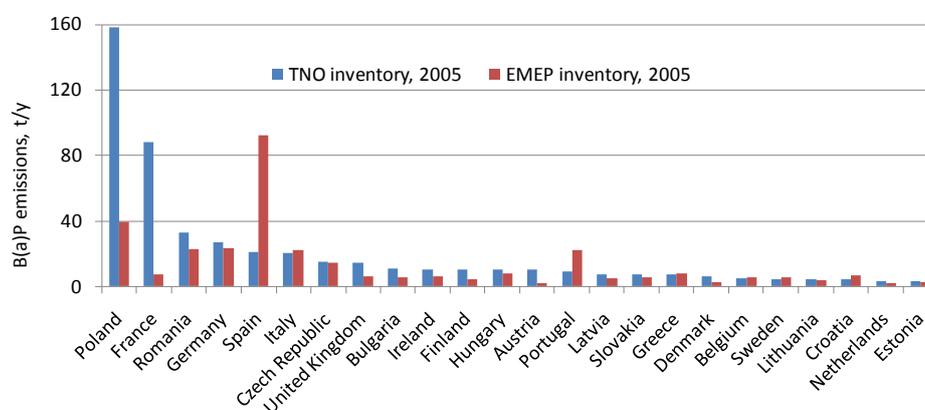
Relative changes of B(a)P emissions in three groups of EMEP countries, namely, EU, non-EU, and the EECCA countries, are shown in Fig.4. Among the EMEP countries more significant decrease is indicated for non-EU countries (-18%) while changes in the EU countries are smaller in this period (-9%). B(a)P emissions in the EECCA countries show increasing tendency (6%).



**Fig. 4.** Relative changes (in %) of total B(a)P emissions from 2000 to 2018 in the EU, non-EU, and EECCA countries (a) and in the particular EU countries (b).

Completeness and accuracy of PAH emissions in the EMEP countries are of particular importance for monitoring of emissions reduction and model assessment of pollution levels in the EMEP region. Officially reported information on PAH emissions is available for about 60% of the EMEP countries (mostly the EU countries), while for other EMEP countries expert estimates of emissions are generated based on various available data [Tista *et al.*, 2017]. Inventories of PAH emissions, reported by the EMEP countries, are characterized by varying level of uncertainties. In order to contribute to the improvement of PAH pollution assessment, evaluation of some aspects related to the consistency of reported national emissions (e.g. total annual emissions, spatial distribution) was performed recently [Gusev *et al.*, 2017; Gusev *et al.*, 2018].

Available expert estimates of PAH anthropogenic emissions provide important information for the analysis of national inventories of PAH/B(a)P emissions reported by the EMEP countries. In particular, official emission data on B(a)P can be compared with the inventory of B(a)P emissions in the EU countries for 2005, prepared by TNO in framework of TRANSPHORM project [Van der Gon *et al.*, 2011]. For more than 60% of the EMEP countries official data on B(a)P emissions (based on the most recent submission of emissions) are rather close to the TNO expert estimates (Fig. 5). At the same time, for some of the countries substantial differences can be noted. In particular, expert estimates of TNO for Poland, France, and Austria are significantly higher than official B(a)P emissions. Opposite situation is seen for Spain and Portugal, where expert estimates are lower comparing to official emissions. Discrepancies found between the TNO and official emission inventories can be used as indication of differences in the methodologies applied by the EMEP countries for the evaluation of PAH emissions.



**Fig. 5.** Officially reported national total B(a)P emissions of EU countries for 2005 in comparison with expert estimates, developed by the TNO in framework of TRANSPHORM project.

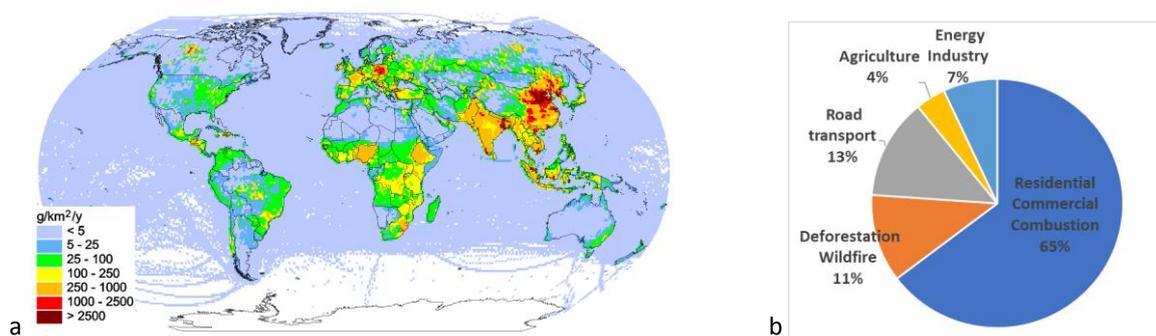
To improve evaluation of pollution in the EMEP countries, further work in cooperation with national expert, CEIP, and TFEIP is required to refine estimates of sector-specific PAH emissions as well as their speciation.

## 4.2. Research-oriented inventories of 16 PAH emissions

Along with the official EMEP emission data a number of research-driven PAH emission inventories were developed using different methodologies. In particular, they include national scale inventory for China [Xu *et al.*, 2006], regional scale inventories for Europe [Van der Gon *et al.*, 2007] and for North America [Galarneau *et al.*, 2007], and global scales inventories [Zhang *et al.*, 2009; Shen *et al.*, 2013].

Some of these inventories provide information on spatial distribution as well as temporal variation of PAH emissions and thus can be applied for studies of long-term trends of pollution and exposure analysis. In particular, the global scale inventory of atmospheric emissions for 16 PAHs has been developed by the research group of Peking University [Shen *et al.*, 2013]. The inventory is based on top-down approach with application of the newly developed fuel consumption database PKU-FUEL-2007 [Wang *et al.*, 2013] and an updated database of PAH emission factors. The inventory covers 16 PAHs, namely, naphthalene (NAP), acenaphthylene (ACY), acenaphthene (ACE), fluorene (FLO), phenanthrene (PHE), anthracene (ANT), fluoranthene (FLA), pyrene (PYR), benzo(a)anthracene (B(a)A), chrysene (CHR), benzo(b)fluoranthene (B(b)F), benzo(k)fluoranthene (B(k)F), benzo(a)pyrene (B(a)P), dibenzo(a,h)anthracene (D(ah)A), indeno(1,2,3-cd)pyrene (I(cd)P), and benzo(g,h,i)perylene (B(g,h,i)P).

Estimates of PAH emissions were disaggregated into  $0.1^\circ \times 0.1^\circ$  resolution global grid. Spatial distribution of 16 PAH annual emissions is given in Fig. 7a. According to these data highest level of PAH emissions took place in the countries of Eastern and Southern Asia. PAH emissions were split into six sectors (energy production, industry, transportation, commercial/residential sources, agriculture, and deforestation/wildfire). In Fig. 7b distribution of global PAH emissions by major source categories is given. The largest contribution to total PAH emissions is made up by Residential and Commercial combustion (65%), followed by Road Transport (13%) as well as Deforestation and Wildfires (11%).



**Fig. 7.** Spatial distribution of global annual emissions of 16 PAHs for 2014 (a) and contribution of major source categories to total PAH emission (b).

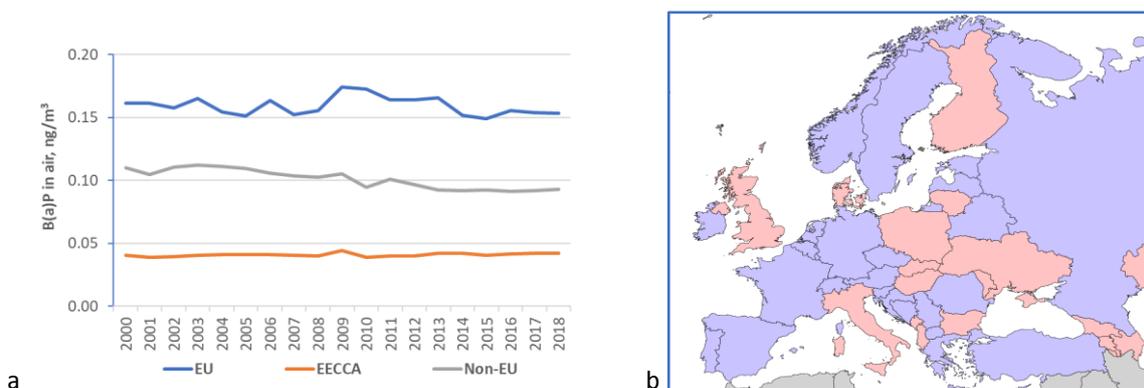
This inventory is applied to study intercontinental transport, spatial and temporal trends and population exposure to mixture of carcinogenic PAHs.

## 5. TEMPORAL VARIATIONS OF PAH POLLUTION LEVELS

The information on trends in pollution levels and exceedances of air quality guidelines can support evaluation of effectiveness of the measures on PAH pollution reduction. PAH pollution levels in the EMEP countries substantially decreased since 1990. The most significant decline took place in the beginning of the 1990s, while during the recent two decades the rate of temporal changes in some parts of the EMEP region has noticeably declined or even levelled off [Gusev *et al.*, 2015]. Analysis of long-term changes of B(a)P pollution in the EMEP region during this period was carried out using the data of EMEP monitoring network and AIRBASE [Gusev *et al.*, 2019]. It was shown that B(a)P concentrations in air demonstrate statistically significant decrease at 30% of the sites and increase at 7% of the sites.

Evaluation of B(a)P pollution temporal variability for the two recent decades was also carried out using the results of model assessment. It was shown that the period 2000-2018 was characterized by generally small changes of annual mean concentrations in the EMEP countries. In particular, according to model predictions average levels of B(a)P concentrations decreased in the EU and non-EU countries by 5% and 15%, respectively, while for the EECCA countries an increase of concentrations by 3% was estimated (Fig. 8a).

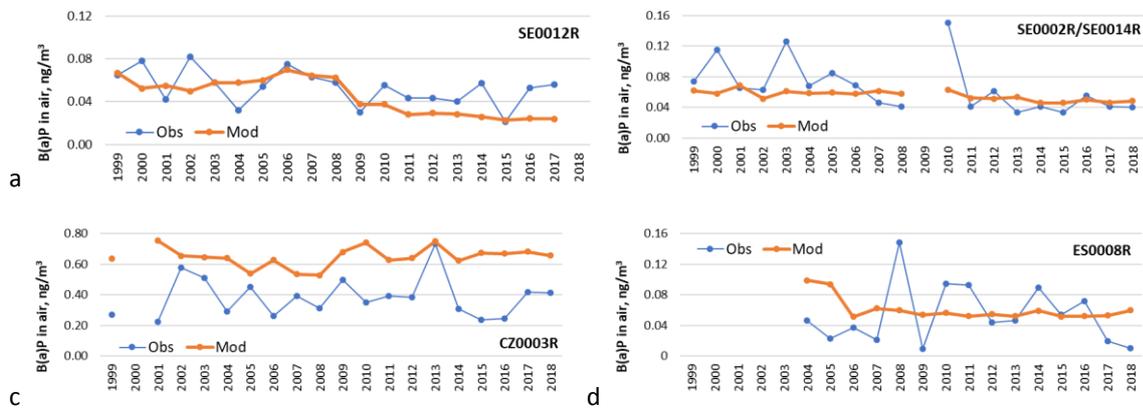
Evaluation of temporal variations of averaged B(a)P concentrations for individual countries showed different directions of changes (Fig. 8b). For about 55% of the EMEP countries a decline of concentrations was predicted. For other EMEP countries (about 45%) increase of B(a)P concentrations was estimated during this period. In particular, increasing concentrations can be noted for some of the countries in Central and Southern Europe (e.g. Poland, Slovakia, Italy) as well as in the other parts of EMEP region (e.g. Finland, United Kingdom).



**Fig. 8.** Temporal changes of average B(a)P annual mean modelled air concentrations from 2000 to 2018 in the EU, EECCA, and non-EU EMEP countries (a). Spatial distribution of changes of averaged B(a)P air concentrations in the EMEP countries for the period 2000-2018. Blue color indicates decrease and red color indicates increase of B(a)P concentrations (b).

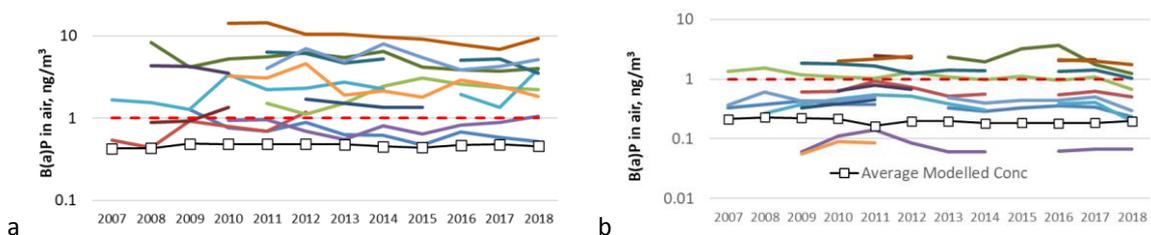
Model estimates of temporal variations of B(a)P pollution in general correspond to long-term measurements of the EMEP monitoring sites. Comparison of annual mean and modelled B(a)P concentrations, predicted by the GLEMOS model, is illustrated on the example of selected monitoring sites in the Fig. 9. According to measurements and model estimates, B(a)P pollution levels

in Sweden and Spain slowly decreased in the period 2000-2018. At the same time pollution levels at background monitoring site CZ0003R in the Czech Republic was almost on the same level during this period.



**Fig. 9.** Comparison of annual mean modelled and observed B(a)P concentrations for the EMEP monitoring sites in Sweden (a,b), the Czech Republic (c), and Spain (d).

Data of national monitoring networks of the AIRBASE provide more detailed information on B(a)P pollution in the EMEP countries. Variability of annual mean B(a)P concentrations observed at rural and background urban monitoring sites in Poland and in Italy is shown in Fig. 10a and b, respectively. Along with measurements, averaged modelled B(a)P concentrations for the selected countries are presented. It can be seen that model predictions and measured concentrations similarly indicate the absence of noticeable decreasing trends in the B(a)P pollution levels in these countries. Some of the monitoring sites show increasing concentrations of B(a)P.



**Fig. 10.** Comparison of average annual mean modelled B(a)P concentrations in Poland (a) and in Italy (b) with measurements of B(a)P at rural and background urban AIRBASE monitoring sites. Colored solid lines indicate observed B(a)P concentrations. Red dotted line indicates the EU target level 1 ng/m³ for B(a)P. Black solid line with squares shows average B(a)P concentrations in the country.

Available data indicate that PAH pollution levels in the EMEP countries during the two recent do not show significant changes. While more than a half of monitoring sites indicate decline of PAH concentrations, part of the monitoring sites demonstrates increasing levels of pollution that requires further analysis. In particular, specific attention at further stages of this work will be given to the statistical significance of changes. Besides, source-receptor relationships should also be accounted for in the analysis of changes. In particular, contributions national and foreign emissions as well as emission sectors to PAH pollution levels will be evaluated to carry out more detailed analysis of temporal trends in PAH air concentrations.

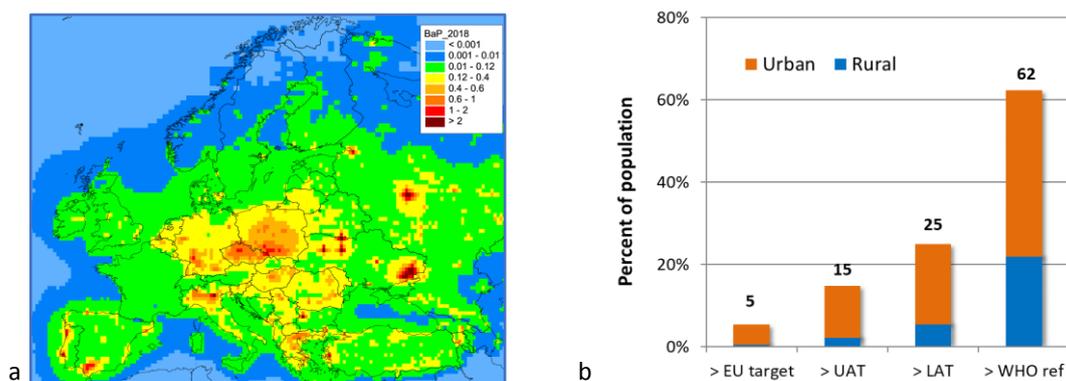
## 6. EVALUATION OF EXPOSURE TO PAHs

The information on exceedances of the EU and WHO air quality guidelines for B(a)P as well as data on B(a)P equivalent air concentrations of toxic PAHs is of importance for the analysis of population exposure to toxic substances and adverse health effects.

### 6.1. Exceedances of B(a)P air quality guidelines

Annual mean B(a)P air concentrations continue to exceed air quality guidelines in some of the areas of the EMEP region. Model predictions for 2018 (Fig.11a) indicate high levels of B(a)P concentrations for the countries of Central and Eastern Europe, e.g. in Poland, the Czech Republic, Bulgaria, northern Italy, Greece, Romania, as well as in some areas of Spain and Turkey. In some of these countries estimates of B(a)P air concentrations exceed the EU air quality guideline. Areas of concentrations above the EU target value are also noted for some of the EECCA countries. However, these estimates are subject of higher uncertainties due to incomplete information on emissions for this part of EMEP region.

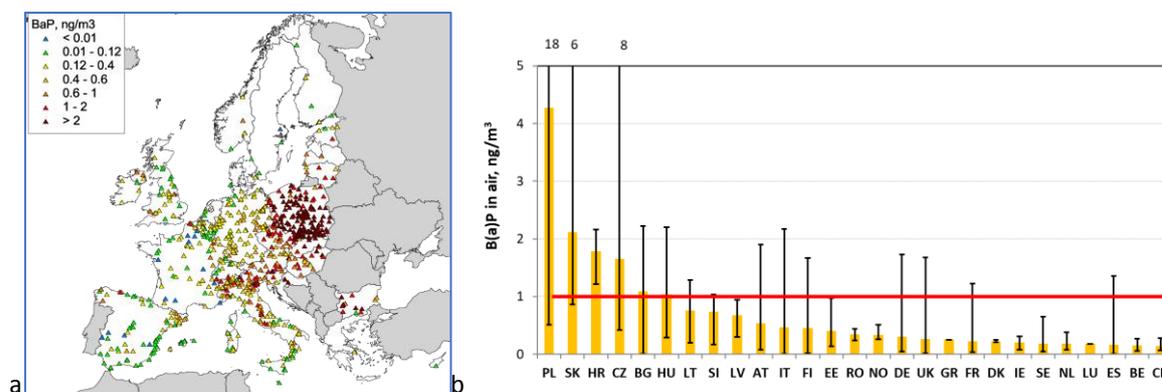
According to modelling results, about 5% of total population of the EMEP countries in 2018 (Fig.11b) were exposed to B(a)P annual mean air concentrations above the EU target level ( $1 \text{ ng/m}^3$ ). Besides, the upper assessment thresholds (UAT) and lower assessment thresholds (LAT) (Directive 2004/107/EC) values were exceeded in the areas with 15% and 25% of population, respectively. It can be seen that most of these exceedances took place for the population of urban areas.



**Fig. 11.** Map of annual mean modelled B(a)P air concentrations for 2018,  $\text{ng/m}^3$  (a) and percentage of urban and rural population of the EMEP countries in the areas with annual mean B(a)P air concentrations above the EU limit values (EU target value for B(a)P –  $1.0 \text{ ng/m}^3$ , UAT –  $0.6 \text{ ng/m}^3$ , LAT –  $0.4 \text{ ng/m}^3$ ), and WHO reference level  $0.12 \text{ ng/m}^3$  (b)

With respect to the WHO reference level, it was estimated that more than 60% of population in the EMEP countries lived in the areas with annual mean B(a)P air concentrations above this limit, while only for less than 40% of population B(a)P concentrations were below the reference level.

Detailed observational data on B(a)P pollution levels are available from national monitoring in the EU countries (AIRBASE). Spatial distribution of observed annual mean B(a)P air concentrations in 2018 is presented in the Fig. 12a. Similar to the modelling results, the highest average B(a)P air concentrations in 2018 were observed at the monitoring stations in Central, Eastern, and Southern Europe (Fig. 12a).



**Fig. 12.** Spatial distribution of B(a)P air concentrations observed at AIRBASE monitoring sites in 2018 (a) and average values of measured annual mean B(a)P air concentrations in the EU countries in 2018 (b). Whiskers denote the range from minimum to maximum of measured concentrations.

Annual mean B(a)P air concentrations observed in 2018 in the selected European countries are illustrated in Fig. 12b. According to these data B(a)P air concentrations, averaged over the monitoring sites of particular country, were above the EU target value in 6 EU countries, namely, Poland, Slovakia, Croatia, the Czech Republic, Bulgaria, and Hungary.

In addition, maximum measured B(a)P concentrations above the EU target value were also reported by some of the monitoring stations in Lithuania, Slovenia, Austria, Italy, Finland, Germany, France, Spain, and the UK. The highest concentrations were measured in the southern part of Poland (more than  $10 \text{ ng}/\text{m}^3$ ). Most of exceedances of the EU target value were observed at the urban background stations.

Exceedances of WHO reference level in 2018 took place in most of the countries performing regular monitoring of B(a)P pollution levels. In particular, annual mean B(a)P concentrations were higher than  $0.12 \text{ ng}/\text{m}^3$  in 27 European countries. Thus, further measures are required to reduce elevated levels of B(a)P concentrations and their adverse effects on population.

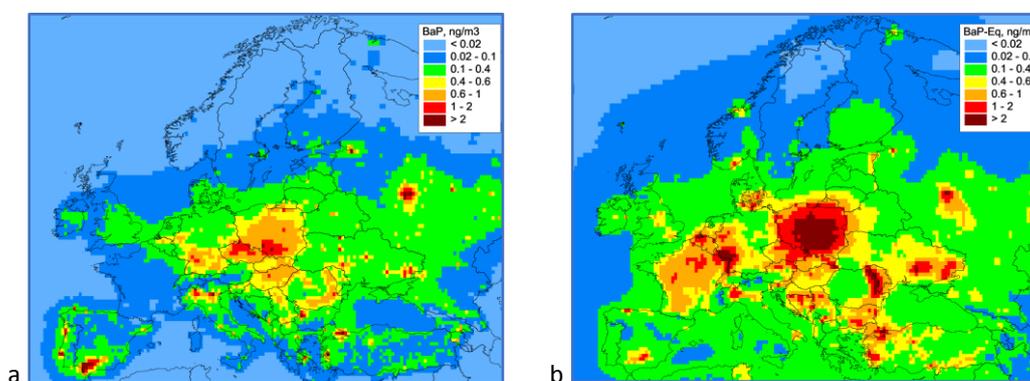
## 6.2. Evaluation of exposure to mixture of 16 PAHs

Evaluation of population exposure to elevated B(a)P air concentrations can be extended by the analysis of other toxic substances of PM chemical composition and evaluation of cumulative human health risk [Liu *et al.*, 2019; Delgado-Saborit *et al.*, 2011]. In particular, atmospheric aerosol particles can be enriched by a mixture of various toxic compounds including other PAHs as well as other POPs (e.g. PCDD/Fs, HCB) and heavy metals.

To evaluate population exposure to mixture of toxic PAH compounds, experimental modelling of 16 EPA PAHs was performed. The set of physical-chemical properties of selected PAHs, necessary to run the GLEMOS model, was prepared on the basis of literature data (Chapter 2). According to collected data on the properties, 8 heavier PAHs present in the atmosphere at ambient temperatures mainly in particulate phase, whereas for other of selected PAHs more significant fraction of gaseous phase can take place. Emission data for model simulations were based on the global gridded emission inventory of PKU (Chapter 4). Model simulations of transboundary pollution and fate of 16 PAHs within the EMEP domain have been carried using nested modelling approach. Boundary conditions for the regional scale simulations were obtained from the GLEMOS model run on a global scale.

Exposure to mixture of toxic PAHs can be estimated using the WHO toxicity equivalency factors defined for individual PAH compounds (TEFs) [ALS, 2013]. These TEFs can be applied to characterize the carcinogenic potency of each considered PAH and calculate B(a)P equivalent concentration of total PAH mixture. B(a)P equivalent concentration of PAH mixture can be calculated as the sum of the products of individual PAH compounds concentrations and their toxic equivalency factors (see equation 1). Thus, B(a)P equivalent concentrations depends both on the TEF values and the emissions.

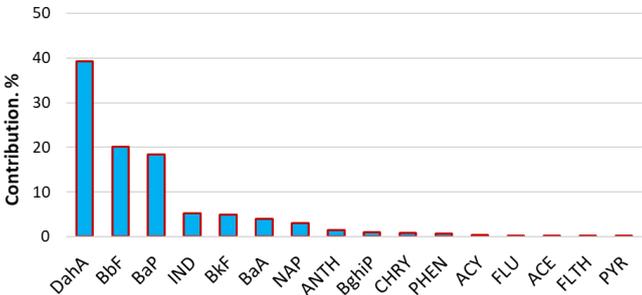
Based on the modelling results for the selected 16 PAHs, B(a)P equivalent concentrations were calculated. The spatial distribution of B(a)P equivalent concentrations of 16 PAHs in comparison to distribution of single B(a)P concentrations are presented in Fig. 13. It can be seen that areas with the exceedances of air quality guidelines in case of B(a)P equivalent concentrations are more significant comparing to the B(a)P concentrations only.



**Fig. 13.** Annual mean modelled B(a)P air concentrations (a) and B(a)P-equivalent air concentrations of 16 PAHs (b) estimated for 2018.

Modelling results make it possible to estimate the contributions of individual 16 compounds to the sum of B(a)P equivalent concentrations (Fig.14). The contribution of particular compounds depends both on the toxic equivalent factor and the levels of their concentrations. It can be seen that the largest contribution to total B(a)P equivalent concentration is made by dibenzo(a,h)anthracene, followed by B(b)F and B(a)P. It can be noted that in spite of relatively high level of toxicity and significant concentrations dibenzo(a,h)anthracene is not currently included in the list of PAHs

considered in the POPs Protocol. Thus, inclusion of additional compounds may help to characterize population exposure to toxic PAHs more accurately.



**Fig. 14.** Contributions of individual 16 PAH compounds to the sum of B(a)P equivalent annual mean concentrations

The information on exceedances of the EU and WHO air quality guidelines for B(a)P as well as data on B(a)P equivalent air concentrations of PAHs are expected to support activities of the Task Force on Health and Working Group on Effects with regard to the analysis of population exposure to toxic substances and their impacts on human health and ecosystems.

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## PHYSICAL-CHEMICAL PROPERTIES OF SELECTED PAHS

The Annex contains information on physical-chemical properties, substance-specific parameters and degradation rates of PAHs in the environmental media, which were used in model parameterization. Description of parameters including forms of temperature dependences were taken out from EMEP/MSC-E Technical Report 5/2005 [Gusev *et al.*, 2005].

### Subcooled liquid-vapour pressure

According to the Junge-Pankow adsorption model, the value of subcooled liquid-vapour pressure ( $p_{OL}$ , Pa) is one of the basic parameters in the modelling of PAH partitioning between its particulate and gaseous phase in air [Junge, 1977; Pankow, 1987]. In addition, the  $p_{OL}$  value have impact on subsequent important processes such as dry and wet deposition and atmospheric degradation [Gusev *et al.*, 2005].

The value of subcooled liquid-vapour pressure ( $p_{OL}$ , Pa) depends on the ambient temperature and is included in the model as follows:

$$p_{OL} = p_{OL}^0 \exp \left[ -a_p \left( \frac{1}{T} - \frac{1}{T_0} \right) \right],$$

where  $T$  is the ambient temperature, K;  $T_0$  is the reference temperature, K;  $p_{OL}^0$  is the value of  $p_{OL}$  at the reference temperature  $T_0$ ;  $a_p$  is the coefficient of the vapour pressure temperature dependence, K.

This formula is obtained from the standard form of the temperature dependence by recalculating the coefficients of the exponential equation:

$$\log p_{OL} (Pa) = -A/T(K) + B$$

using the following formulas:

$$a_p = A \cdot \ln(10)$$

$$p_{OL}^0 = 10^{-A/T_0+B}$$

The coefficients of  $p_{OL}$  temperature dependence and base values given at the temperature 283.15 K ( $T_0$ ) for the selected PAHs are listed in Table A.1.

**Table A.1.** Coefficients of  $p_{OL}$  temperature dependence used in model parameterization

Substance	Value					Log $p_{OL}$ (298 K)	Reference
	$T_0$	A	B	$p_{OL}^0$	$a_p$		
Benzo(a)pyrene	283.15	6060	14.864	2.8968E-07	13953.6657	-5.461	Allen et al., 1999
Benzo(a)anthracene	283.15	3731	8.864	4.8667E-05	8590.94498	-3.648	Allen et al., 1999
Dibenzo(a,h)anthracene	283.15	7009	16.378	4.2105E-09	16138.8189	-7.129	Allen et al., 1999
Benzo(b)fluoranthene	283.15	4578	9.48	2.0506E-07	10541.2346	-5.875	Paasivirta et al., 1999
Benzo(k)fluoranthene	283.15	4427	9.48	7.0013E-07	10193.5442	-5.368	Paasivirta et al., 1999
Chrysene	283.15	5676	14.663	4.1408E-06	13069.473	-4.374	Allen et al., 1999
Indeno(1,2,3-cd)pyrene	283.15	4839	9.60	3.2368E-08	11142.2093	-6.630	Paasivirta et al., 1999
Acenaphthylene	283.15	2751	9.53	0.0012495	8445.882	-2.252	Paasivirta et al., 1999
Fluoranthene	283.15	3668	10.051	0.0012495	8445.88212	-2.252	Allen et al., 1999
Pyrene	283.15	4067	11.260	0.00078811	9364.61357	-2.382	Allen et al., 1999
Naphthalene	283.15	3075	11.835	9.44129973	7080.44916	1.518	Allen et al., 1999
Fluorene	283.15	3779	12.330	0.09632014	8701.46907	-0.347	Allen et al., 1999
Acenaphthene	283.15	3561	12.073	0.3137813	8199.50552	0.129	Allen et al., 1999
Benzo(g,h,i)perylene	283.15	6707	10.487	6.3082E-14	15443.4382	-12.010	Allen et al., 1999
Anthracene	283.15	3667	11.015	0.0115949	8443.57954	-1.285	Allen et al., 1999
Phenanthrene	283.15	4297	13.177	0.01002993	9894.20814	-1.237	Allen et al., 1999

## Henry's law constant and air/water partition coefficient

The value of the Henry's law constant and the air/water partition coefficient are used to describe the process of gas exchange between the atmosphere and soil, the atmosphere and seawater, as well as wet deposition of gaseous phase of PAHs [Gusev et al., 2005]. The ratio between the Henry's law constant,  $K_H$ , (Pa·m<sup>3</sup>/mol) and the air/water partition coefficient  $K_{aw}$ , (dimensionless) is as follows:

$$K_{aw} = K'_H = \frac{K_H}{RT}$$

where  $T$  - temperature, K;  $R = 8.314$  J/(mol·K) - universal gas constant.

The temperature dependence of the Henry's law constant  $K'_H$  (dimensionless) is used in the model parameterization, as follows:

$$K'_H = \frac{K_{H0}}{RT} \exp \left[ -a_H \left( \frac{1}{T} - \frac{1}{T_0} \right) \right]$$

where  $T$  is the ambient air temperature, K;  $T_0$  is the reference temperature;  $R$  is the universal gas constant, J/(mol·K),  $a_H$  is the coefficient of Henry's law constant temperature dependence, K;  $K_{H0}$  is the value of Henry's law constant at reference temperature, Pa·m<sup>3</sup>/mol.

This formula is obtained from the standard form of the temperature dependence by recalculating the coefficients of the exponential equation

$$\log K_H (\text{Pa} \cdot \text{m}^3/\text{mol}) = -A/T(K) + B$$

using the following formulas:

$$a_H = A \cdot \ln(10)$$

$$K_{HO} = 10^{-A/T_0+B}$$

Coefficients of the temperature dependence of the Henry's law constant for the selected POPs are presented in Table A.2.

**Table A.2.** Coefficients of temperature dependence of Henry's law constant used in model parameterization

Substance	Value			$K_{HO}$	$a_H$	$\log K_H$ (298.15 K)	Ref
	$T_0$	A	B				
Benzo(a)pyrene	283.15	3373.71	10.5985	0.048259	7768.254	-0.71698	<i>Parnis et al., 2015</i>
Benzo(a)anthracene	283.15	3222.02	10.4494	0.117544	7418.975	-0.35731	<i>Parnis et al., 2015</i>
Dibenzo(a,h)anthracene	283.15	3804.62	11.3258	0.007745	8760.461	-1.43496	<i>Parnis et al., 2015</i>
Benzo(b)fluoranthene	283.15	3438.16	10.7422	0.03978	7916.656	-0.78945	<i>Parnis et al., 2015</i>
Benzo(k)fluoranthene	283.15	3457.54	10.8171	0.040375	7961.28	-0.77955	<i>Parnis et al., 2015</i>
Chrysene	283.15	3204.84	10.3614	0.110376	7379.417	-0.38769	<i>Parnis et al., 2015</i>
Indeno(1,2,3-cd)pyrene	283.15	3613.54	10.9810	0.01656	8320.483	-1.13887	<i>Parnis et al., 2015</i>
Acenaphthylene	283.15	2271.52	8.8156	6.21269	5230.368	1.196885	<i>Parnis et al., 2015</i>
Fluoranthene	283.15	2850.20	9.7903	0.529977	6562.828	0.230682	<i>Parnis et al., 2015</i>
Pyrene	283.15	2780.21	9.6440	0.668561	6401.67	0.31913	<i>Parnis et al., 2015</i>
Naphthalene	283.15	2004.90	8.4590	23.89465	4616.453	1.734532	<i>Parnis et al., 2015</i>
Fluorene	283.15	2482.51	9.3181	3.55326	5716.191	0.991721	<i>Parnis et al., 2015</i>
Acenaphthene	283.15	2250.90	9.0081	11.44467	5182.889	1.458544	<i>Parnis et al., 2015</i>
Benzo(g,h,i)perylene	283.15	3525.61	10.7566	0.020194	8118.017	-1.06835	<i>Parnis et al., 2015</i>
Anthracene	283.15	2620.30	9.4938	1.736578	6033.464	0.705271	<i>Parnis et al., 2015</i>
Phenanthrene	283.15	2606.56	9.4130	1.612204	6001.826	0.670555	<i>Parnis et al., 2015</i>

## Washout ratio

The model separately considers the wet deposition of gaseous and particulate phases of PAHs.

In regard to the leaching of the gaseous phase of PAHs with precipitation, it is assumed in the model that the equilibrium between the vapor phase and the dissolved phase in the raindrop is reached rapidly, and the washout ratios for the gaseous phase ( $W_g$  dimensionless) of PAHs is determined as inverse values to dimensionless Henry's law constant:

$$W_g = \frac{1}{K'_H}$$

where  $K'_H$  is the dimensionless Henry's law constant.

It should be noted, that the values of the washout ratios for the gaseous phase of PAHs can also be determined experimentally based on the relationship of a compound concentration in the dissolved phase in wet depositions and in the gaseous phase in

In regard to the leaching of the particle bound phase of PAHs with precipitation ( $W_p$ , dimensionless), the values of the washout ratio which are determined experimentally or obtained theoretically can be used. Wet deposition of particulate phase of PAHs is the prevailing mechanism of removing of pollutants that occur in the air predominantly associated with the particles.

Table A.3 gives washout ratio values of the considered PAHs used in the model parameterization.

**Table A.3.** Washout ratio, used in the model parameterization

Substance	$W_p$ , dimensionless	References
Benzo(a)pyrene	$3.0 \cdot 10^3$ (Range 7.2 - $1.4 \cdot 10^6$ )	<i>Skrdlíková et al, 2011</i>
Benzo(a)anthracene	$4.3 \cdot 10^3$ (Range 47- $9.1 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>
Dibenzo(a,h)anthracene	$2.2 \cdot 10^3$ (Range 290- $5.1 \cdot 10^6$ )	<i>Skrdlíková et al, 2011</i>
Benzo(b)fluoranthene	$1.5 \cdot 10^4$ (Range 8.8- $9.4 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>
Benzo(k)fluoranthene	$2.0 \cdot 10^4$ (Range 24- $8.1 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>
Chrysene	$1.5 \cdot 10^4$ (Range 94- $8.0 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>
Indeno(1,2,3-cd)pyrene	$6.2 \cdot 10^3$ (Range 28- $1.6 \cdot 10^7$ )	<i>Skrdlíková et al, 2011</i>
Acenaphthylene	$2.1 \cdot 10^3$ (Range 61- $1.7 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>
Fluoranthene	$2.0 \cdot 10^4$ (Range 3000- $4.7 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>
Pyrene	$1.3 \cdot 10^4$ (Range 50- $3.8 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>
Naphthalene	$2.7 \cdot 10^7$	<i>He &amp; Balasubramanian, 2009</i> <i>Zhang et al, 2015</i>
Fluorene	$1.6 \cdot 10^4$ (Range 34- $4.3 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>
Acenaphthene	$5.5 \cdot 10^3$ (Range 32- $4.7 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>
Benzo(g,h,i)perylene	$1.8 \cdot 10^5$	<i>He &amp; Balasubramanian, 2009</i>
Anthracene	$6.3 \cdot 10^3$ (Range 62- $1.7 \cdot 10^6$ )	<i>Skrdlíková et al, 2011</i>
Phenanthrene	$1.8 \cdot 10^4$ (Range 550- $4.2 \cdot 10^5$ )	<i>Skrdlíková et al, 2011</i>

## Degradation rate constants in environmental media

Degradation process of PAHs in the atmosphere includes the gas-phase reactions and degradation of PAHs associated with particles with hydroxyl radicals, ozone and  $\text{NO}_3$  radicals. These reactions are described by the equation:

$$\frac{dC}{dt} = -k_{air} \cdot C \cdot [reactant],$$

where  $C$  is the pollutant concentration in air,  $\text{ng/m}^3$ ;  $[reactant]$  is concentration of considered reactant,  $\text{molec/cm}^3$ .

Values of second order degradation rate constants in air ( $k_{air}$ ), used in model parameterization are presented in Table A.4.

**Table A.4.** Degradation rate constants in air  $k_{air}$ , used in model parameterization

Substance	Gaseous			Particles		
	$k_{g\ OH}, \text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$	$k_{g\ O_3}, \text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$	$k_{g\ NO_3}, \text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$	$k_{OH}, \text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$	$k_{O_3}, \text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$	$k_{NO_3}, \text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$
Benzo(a)pyrene	$3.5 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>		$5.4 \cdot 10^{-11}$ <i>Lammel et al., 2009</i>	$4.1 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$5.3 \cdot 10^{-17}$ <i>Keyte et al., 2013</i>	$2.6 \cdot 10^{-17}$ <i>Lammel et al., 2009</i>
Benzo(a)anthracene	$50 \cdot 10^{-12}$ *			$5.6 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$2.8 \cdot 10^{-17}$ <i>Keyte et al., 2013</i>	
Dibenzo(a,h)anthracene	$50 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>			$1.6 \cdot 10^{-14}$ <i>Keyte et al., 2013</i>		
Benzo(b)fluoranthene	$16 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>			$1.2 \cdot 10^{-14}$ <i>Keyte et al., 2013</i>		
Benzo(k)fluoranthene	$54 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>			$3.5 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$1.9 \cdot 10^{-17}$ <i>Keyte et al., 2013</i>	
Chrysene	$50 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>			$5.0 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$1.5 \cdot 10^{-17}$ <i>Keyte et al., 2013</i>	$4.0 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>
Indeno(1,2,3-cd)pyrene	$64 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>			$3.5 \cdot 10^{-13}$ <i>Keyte et al., 2013</i>	$1.9 \cdot 10^{-17}$ <i>Keyte et al., 2013</i>	
Acenaphthylene	$110 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$5.5 \cdot 10^{-16}$ <i>Keyte et al., 2013</i>	$7.96 \cdot 10^{-24}$ <i>Keyte et al., 2013</i>			
Fluoranthene	$50 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>		$5.1 \cdot 10^{-28}$ <i>Keyte et al., 2013</i>	$3.2 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>	$1.9 \cdot 10^{-17}$ <i>Keyte et al., 2013</i>	$4.0 \cdot 10^{-19}$ <i>Lammel et al., 2009</i>
Pyrene	$50 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>		$1.6 \cdot 10^{-27}$ <i>Keyte et al., 2013</i>	$3.1 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$2.5 \cdot 10^{-17}$ <i>Keyte et al., 2013</i>	$6.4 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>
Naphthalene	$23 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$<0.3 \cdot 10^{-18}$ <i>Keyte et al., 2013</i>	$3.3 \cdot 10^{-28}$ <i>Keyte et al., 2013</i>	$5 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$0.9 \cdot 10^{-18}$ <i>Keyte et al., 2013</i>	
Fluorene	$13 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>		$5.1 \cdot 10^{-26}$ <i>Keyte et al., 2013</i>	$3.1 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>		
Acenaphthene	$100 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$<0.5 \cdot 10^{-18}$ <i>Keyte et al., 2013</i>	$1.7 \cdot 10^{-27}$ <i>Keyte et al., 2013</i>			
Benzo(g,h,i)perylene	$87 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>			$5.9 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>		
Anthracene	$17 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>			$4.4 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$9.8 \cdot 10^{-17}$ <i>Keyte et al., 2013</i>	$9.0 \cdot 10^{-19}$ <i>Lammel et al., 2009</i>
Phenanthrene	$13 \cdot 10^{-12}$ <i>Lammel et al., 2015</i>	$4.0 \cdot 10^{-19}$ <i>Keyte et al., 2013</i>	$1.74 \cdot 10^{-25}$ <i>Keyte et al., 2013</i>	$5.0 \cdot 10^{-12}$ <i>Keyte et al., 2013</i>	$2.4 \cdot 10^{-17}$ <i>Keyte et al., 2013</i>	

The degradation process of PAHs in soil is described in the model as a first-order process as follows:

$$\frac{dC}{dt} = -k_{soil}C,$$

where  $C$  is the concentration of substance in soil,  $\text{ng}/\text{m}^3$ ;  $k_{soil}$  is the degradation rate constant for soil,  $\text{s}^{-1}$ .

For seawater, the degradation process of PAHs can be described also as a first-order process by following equation:

$$\frac{dC}{dt} = -k_{sea}C,$$

where  $C$  is the concentration of substance in seawater,  $\text{pg}/\text{L}$ ;  $k_{sea}$  is the degradation rate constant for seawater,  $\text{s}^{-1}$ .

Values of the degradation rate constants in soil and seawater for the considered PAHs are presented in Table A.5.

**Table A.5.** Degradation rate constants in environmental media  $k_{soil}$  and  $k_{sea}$  used in model parameterization

Substance	$k_{soil}, \text{s}^{-1}$	$k_{sea}, \text{s}^{-1}$	References
Benzo(a)pyrene	$1.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-7}$	Mackay et al., 2006
Benzo(a)anthracene	$1.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-7}$	Mackay et al., 2006
Dibenzo(a,h)anthracene	$1.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-7}$	Mackay et al., 2006
Benzo(b)fluoranthene	$1.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-7}$	Mackay et al., 2006
Benzo(k)fluoranthene	$1.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-7}$	Mackay et al., 2006
Chrysene	$1.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-7}$	Mackay et al., 2006
Indeno(1,2,3-cd)pyrene	$1.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-7}$	Mackay et al., 2006
Acenaphthylene	$1.34 \cdot 10^{-7}$	$1.34 \cdot 10^{-7}$	Mackay et al., 2006
Fluoranthene	$1.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-7}$	Mackay et al., 2006
Pyrene	$1.13 \cdot 10^{-8}$	$1.13 \cdot 10^{-7}$	Mackay et al., 2006
Naphthalene	$1.13 \cdot 10^{-7}$	$1.13 \cdot 10^{-6}$	Mackay et al., 2006
Fluorene	$3.5 \cdot 10^{-8}$	$3.5 \cdot 10^{-7}$	Mackay et al., 2006
Acenaphthene	$3.5 \cdot 10^{-8}$	$3.5 \cdot 10^{-7}$	Mackay et al., 2006
Benzo(g,h,i)perylene	$1.36 \cdot 10^{-8}$	$1.36 \cdot 10^{-8}$	Mackay et al., 2006
Anthracene	$3.5 \cdot 10^{-8}$	$3.5 \cdot 10^{-7}$	Mackay et al., 2006
Phenanthrene	$3.5 \cdot 10^{-8}$	$3.5 \cdot 10^{-7}$	Mackay et al., 2006

## Octanol-water partition coefficient

The octanol-water partition coefficient ( $K_{OW}$ , dimensionless) is a characteristic of the hydrophobicity of a substance. It describes the distribution of the compound between water and the lipid medium.  $K_{OW}$  can be used also for the estimation of the partition coefficient in the organic carbon-water system ( $K_{OC}$ ), and for the calculation of the bioconcentration factor (BCF).

For the considered PAHs partition coefficients in the “octanol-water” system selected for modelling are given in Table A.6.

**Table A.6.** Octanol-water partition coefficient ( $K_{OW}$ ), dimensionless used in the model parameterization

Substance	$\log K_{OW}$	$K_{OW}$	References
Benzo(a)pyrene	6.50	3.16E+06	Lammel et al., 2015
Benzo(a)anthracene	5.61	4.07E+05	Lammel et al., 2015
Dibenzo(a,h)anthracene	6.5	$3.16 \cdot 10^6$	Lammel et al., 2015
Benzo(b)fluoranthene	6.12	1.32E+06	Lammel et al., 2015
Benzo(k)fluoranthene	6.84	6.92E+06	Lammel et al., 2015
Chrysene	5.91	8.13E+05	Lammel et al., 2015
Indeno(1,2,3-cd)pyrene	6.58	3.80E+06	Lammel et al., 2015
Acenaphthylene	4.07	1.17E+04	Lammel et al., 2015
Fluoranthene	5.20	$0.16 \cdot 10^6$	LOG KOW Databank, compiled by Dr. James Sangster, Canada
Pyrene	5.18	1.51E+05	Lammel et al., 2015
Naphthalene	3.37	2344	Lammel et al., 2015
Fluorene	4.18	15136	Lammel et al., 2015
Acenaphthene	3.92	8317	Lammel et al., 2015
Benzo(g,h,i)perylene	6.63	$4.27 \cdot 10^6$	Lammel et al., 2015
Anthracene	4.50	31623	Lammel et al., 2015
Phenanthrene	4.60	39811	Lammel et al., 2015

## Octanol-air partition coefficient

The octanol-air partition coefficient ( $K_{OA}$ , dimensionless) is used to describe the distribution of the substance between air and the cuticle of plants, between the gaseous phase and the organic film of atmospheric aerosol particles, etc.  $K_{OA}$  can be defined experimentally (by the ratio of equilibrium concentrations of a substance in octanol and air) or through using of coefficients “octanol-water” ( $K_{OW}$ ) and “air-water” ( $K_{AW}$ ).

Octanol-air partition coefficient ( $K_{OA}$ ) depends on temperature of ambient air. The temperature dependence of partition coefficient in the “octanol-air” system is expressed in the following form:

$$K_{OA} = K_{OA}^0 \exp \left[ a_k \left( \frac{1}{T} - \frac{1}{T_0} \right) \right]$$

where  $T_0 = 283.15$  K is the reference temperature;  $K_{OA}^0$  is the  $K_{OA}$  value at the reference temperature;  $T_0, K, a_k$  is the coefficient of  $K_{OA}$  temperature dependence, K.

Coefficients for  $K_{OA}$  temperature dependence of the considered PAHs used for modelling are presented in Table A.7.

**Table A.7.** Octanol-air partition coefficient ( $K_{OA}$ ), dimensionless used in the model parameterization

Substance	Value					Reference
	$T_0$	A	B	$a_k$	$K_{OA}^0$	
Benzo(a)pyrene	283.15	5382	-6.5	12392	$3.22 \cdot 10^{12}$	Odabasi et al., 2006
Benzo(a)anthracene	283.15	4746	-5.64	10928	$1.32 \cdot 10^{11}$	Odabasi et al., 2006
Dibenzo(a,h)anthracene	283.15	5887	-7.17	13555	$4.18 \cdot 10^{13}$	Odabasi et al., 2006
Benzo(b)fluoranthene	283.15	5285	-6.40	12169	$1.84 \cdot 10^{12}$	Odabasi et al., 2006
Benzo(k)fluoranthene	283.15	5301	-6.42	12206	$2.0 \cdot 10^{12}$	Odabasi et al., 2006
Chrysene	283.15	4754	-5.65	10946	$1.38 \cdot 10^{11}$	Odabasi et al., 2006
Indeno(1,2,3-cd)pyrene	283.15	5791	-7.00	13334	$2.83 \cdot 10^{13}$	Odabasi et al., 2006
Acenaphthylene	283.15	2476	-1.97	5701	$5.94 \cdot 10^6$	Odabasi et al., 2006
Fluoranthene	283.15	3904	-4.34	8989	$2.80 \cdot 10^9$	Odabasi et al., 2006
Pyrene	283.15	3985	-4.56	9175	$3.26 \cdot 10^9$	Chen et al., 2018
Naphthalene	283.15					
Fluorene	283.15	2833	-2.61	6523	$2.48 \cdot 10^7$	Odabasi et al., 2006
Acenaphthene	283.15	2597	-2.20	5970	$9.37 \cdot 10^6$	Odabasi et al., 2006
Benzo(g,h,i)perylene	283.15	5834	-7.03	13433	$3.75 \cdot 10^{13}$	Odabasi et al., 2006
Anthracene	283.15	3316	-3.41	7635	$2 \cdot 10^8$	Odabasi et al., 2006
Phenanthrene	283.15	3293	-3.37	7582	$1.81 \cdot 10^8$	Odabasi et al., 2006

## Molecular diffusion coefficients in air and water

Molecular diffusion coefficients ( $D_A, D_W, \text{m}^2/\text{s}$ ) are used in the description of the PAH air-soil exchange process. The molecular diffusion coefficient of an organic compound in air ( $D_A, \text{m}^2/\text{s}$ ) can be estimated by the formula [Schwarzenbach et al., 1993]:

$$D_A = 10^{-7} \cdot \frac{T^{1.75} * \left[ \frac{1}{M_{air}} + \frac{1}{M} \right]^{0.5}}{p \cdot [\bar{V}_{air}^{1/3} + \bar{V}_m^{1/3}]^2}$$

where  $T$  is the absolute temperature, 298 K;  $M_{air}$  is the mean molecular air weight,  $\sim 29$  g/mol;  $M$  is the molecular weight of an organic substance, g/mol;  $p$  is the pressure, 1 atm;  $\bar{V}_{air}$  is the mean molar gas volume in the air,  $\sim 20.1$  cm<sup>3</sup>/mol;  $\bar{V}_m$  is the molar volume of an organic substance, cm<sup>3</sup>/mol.

For the determination of molecular diffusion coefficients for organic substances in water ( $D_w$ , m<sup>2</sup>/s), the following ratio [Schwarzenbach *et al.*, 1993] can be used:

$$D_w = \frac{13.26 \cdot 10^{-9}}{\mu^{1.14} \cdot \bar{V}_m^{0.589}}$$

where  $\mu$  is the solution viscosity in centipoise at a certain temperature, taken to be equal to water viscosity, 0.894 cps at 298K;  $\bar{V}_m$  is the mean molar volume of a substance, cm<sup>3</sup>/mol.

Table A.8 contains values of molecular diffusion coefficients for air and water as well as molar volume and molar masses of considered PAHs.

**Table A.8.** Molecular diffusion coefficients in air and water, m<sup>2</sup>/s used in the model parameterization

Substance	M, g/mol	V <sub>m</sub> , cm <sup>3</sup> /mol	D <sub>a</sub> , m <sup>2</sup> /s	D <sub>w</sub> , m <sup>2</sup> /s	References
Benzo(a)pyrene	252.31	263	5.032 × 10 <sup>-6</sup>	5.658 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Benzo(a)anthracene	228.29	212.9	5.579 × 10 <sup>-6</sup>	6.408 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Dibenzo(a,h)anthracene	278.36	300.0	4.707 × 10 <sup>-6</sup>	5.236 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Benzo(b)fluoranthene	252.31	268.9	4.980 × 10 <sup>-6</sup>	5.585 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Benzo(k)fluoranthene	252.31	268.9	4.980 × 10 <sup>-6</sup>	5.585 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Chrysene	228.29	251.0	5.171 × 10 <sup>-6</sup>	5.816 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Indeno(1,2,3-cd)pyrene	276.33	233.8	5.292 × 10 <sup>-6</sup>	6.064 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Acenaphthylene	152.19	141.2	6.893 × 10 <sup>-6</sup>	8.161 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Fluoranthene	202.26	217.0	5.571 × 10 <sup>-6</sup>	6.336 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Pyrene	202.25	214.0	5.607 × 10 <sup>-6</sup>	6.389 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Naphthalene	128.17	147.6	6.861 × 10 <sup>-6</sup>	7.951 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Fluorene	166.23	188.0	6.027 × 10 <sup>-6</sup>	6.895 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Acenaphthene	154.21	173.0	6.293 × 10 <sup>-6</sup>	7.241 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Benzo(g,h,i)perylene	276.33	277.0	4.889 × 10 <sup>-6</sup>	5.488 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Anthracene	178.23	197.0	5.871 × 10 <sup>-6</sup>	6.708 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006
Phenanthrene	178.23	199.0	5.845 × 10 <sup>-6</sup>	6.668 × 10 <sup>-10</sup>	Mackay <i>et al.</i> , 2006