

EMEP CONTRIBUTION TO THE PREPARATORY WORK  
FOR THE REVIEW OF THE CLRTAP PROTOCOL ON  
PERSISTENT ORGANIC POLLUTANTS

NEW SUBSTANCES:

Model assessment of potential for long-range  
transboundary atmospheric transport and persistence of  
Polychlorinated Naphthalenes

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## INTRODUCTION

Polychlorinated naphthalenes (PCNs) are a group of compounds composed of two fused benzene rings with one to eight chlorine substitutions. Their molecular structures are similar to those of PCDD/Fs and PCBs. Several of the higher chlorinated congeners are found to elicit biochemical responses similar to the toxic 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) [Lundgren *et al.*, 2003]. A quantitative assessment of dioxin-like potential of PCN congeners has been performed in several studies [Hanberg *et al.*, 1990, Blankenship *et al.*, 1999; Villeneuve *et al.*, 2000; Blankenship *et al.*, 2000, etc].

Due to chemical and thermal stability, good electrical insulation properties, excellent weather resistance and low flammability, PCNs were manufactured as several different technical formulations and widely used in electrical and electronic equipment [Järnberg *et al.*, 1997]. Besides, several emission sources of PCNs in the environment have been suggested apart from those associated with the production and continued use of these formulations. In particular, PCNs are usually common impurities found in technical PCB mixtures and they are formed in thermal (e.g. combustion, roasting, metal reclamation) and other processes (e.g. chloro-alkali industry) in the presence of chlorine [Falandysz, 1998].

PCNs are included into the OSPAR List of Chemicals for Priority Action (Update 2004) [Meeting of the OSPAR Commission (OSPAR), 2004]. As potential candidates for the inclusion into the UN ECE Protocol on POPs this group of compounds was addressed by the Ad Hoc Expert Group on POPs [Lerche *et al.*, 2002]. This year the European Commission has submitted a proposal for amendment to the Protocol with regard to PCNs. In accordance with a suggestion of the Working Group on Strategies and Review that during the 90-day period between the submission of dossier and the twenty-third session of the Executive Body, the dossier on PCNs prepared by national experts [van de Plassche and Schwegler, 2002] is available on the Convention's website for comment and submission of additional information by all interested persons or groups. Additional information for the evaluation of PCNs as potential new POPs in accordance with the two criteria: potential for long-range transboundary atmospheric transport (LRTP) and persistence can be provided by modelling.

A certain experience in the model assessment of the long-range transboundary atmospheric transport and persistence in the environment for a wide range of typical POPs already included in the Protocol on POPs and some potential new POPs [Shatalov *et al.*, 2003; Dutchak *et al.*, 2004; Mantseva *et al.*, 2004; Vulykh *et al.*, 2004, 2005] is accumulated in the Meteorological Synthesizing Centre-East of EMEP. For the evaluation of LRTP and persistence of PCNs, EMEP/MSCE-POP multicompartiment hemispheric transport model is used. Taking into account that PCN group includes 75 possible congeners; this model assessment is carried out for PCN-47. This congener was selected as a representative of the most widespread group of tetra-chlorinated naphthalenes (tetra-CNs) in PCN congener profiles of environmental and source related samples. The homological group of tetra-CNs was detected in most types of samples in prevalent quantities (see Annex A). To estimate LRTP and persistence for PCN-47, the model calculation of its atmospheric transport from a conventional emission point source located in Europe (10°E; 47.5°N) is made for one-year period. Information on physical-chemical properties and degradation rates of this pollutant used for modelling is presented in Annex B.

To illustrate LRTP of the considered congener of tetra-CNs, two numerical characteristics are calculated. The first one is residence time in the atmosphere (**Half-life in air**<sub>calc</sub> ( $T_{1/2}^{air}$ )) obtained with allowance of all processes removing the considered pollutant from the atmosphere. The second is **Transport Distance (TD)** that is the distance from the source at which annual mean atmospheric

concentration of a chemical in question drops 1000 times compared with the concentration near the source. Additional information on this criterion for PCN-47 is provided by the spatial distribution of air pollution caused by the considered conventional point source.

Persistence in the environment is evaluated by **Half-life in the environment** ( $T_{1/2}^{env}$ ) estimated for PCN-47 on the basis of the model simulation of its atmospheric transport taking into account deposition processes, degradation and exchange of the pollutant between main environmental media.

To diminish uncertainties in evaluating LRTP and persistence of the considered congener of PCNs with the help of the model dependent  $TD$  and  $T_{1/2}^{env}$ , a comparison of their numerical values against those obtained for B[a]P as an adequately studied “benchmark substance” is presented.

In conclusion, the calculated numerical characteristics of LRTP and persistence of PCN-47 are given in relation to the indicative criteria outlined in Executive Body Decision 1998/2.

Detailed information on the structure of the model and parameterisation of the media processes can be found in the EMEP/MSCE reports [Gusev *et al.*, 2005] and on the Internet (<http://www.msceast.org>).

## 1. LONG-RANGE TRANSPORT POTENTIAL

According to the Executive Body Decision 1998/2 the LRTP criterion for the evaluation of new substances as potential candidates for the inclusion into the Protocol on POPs is characterized by indicative numerical values of their vapour pressure and atmospheric half-life, which should be greater than two days.

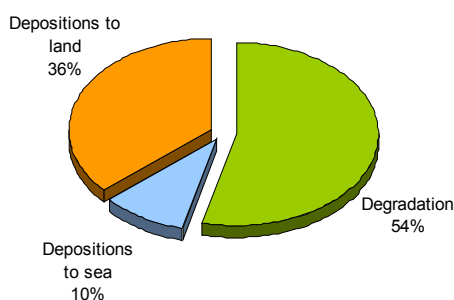
The half-life of “new substances” in the atmosphere can be estimated with the help of modelling as residence time in the atmosphere (*Half-life in air<sub>calc</sub>* ( $T_{1/2}^{air}$ )) obtained on the basis of simulation of their atmospheric transport taking into account not only degradation process in this medium but also all other removal processes. Advantages of modelling approach are contained in possibility to distinguish the most important processes affecting LRTP of a particular considered pollutant in the atmosphere. Additional information on LRTP based also on the model calculations of atmospheric transport is provided by the spatial distribution of air pollution. The latter allows us to estimate *Transport Distance* ( $TD$ ), characterising LRTP of “new substances” as the distance from the source at which annual mean atmospheric concentration drops 1000 times compared with the concentration near the source.

This Chapter contains the main results on evaluation of LRTP criterion for PCN-47 with the help of above-mentioned characteristics obtained on the basis of the EMEP/MSCE-POP model calculations performed at the hemispheric level.

### 1.1. Residence time in the atmosphere

To estimate the residence time in the atmosphere, the model calculation of PCN atmospheric transport with allowance of such processes as degradation in the atmosphere, partitioning between particulate and gas phases, dry and wet deposition of particles and gas exchange with various types of underlying surface is carried out. Emissions of PCN-47 to the atmosphere are assumed to be 1 tonne per year from a conventional point emission source located in Europe (10°E; 47.5°N). On the

basis of this calculation annual atmospheric balance of the considered congener of PCNs emitted to the atmosphere is estimated. The calculated balance for the processes of PCN-47 removal from the atmosphere is given in Fig.1.



*Fig.1. Calculated annual balance of PCN-47 removal from the atmosphere*

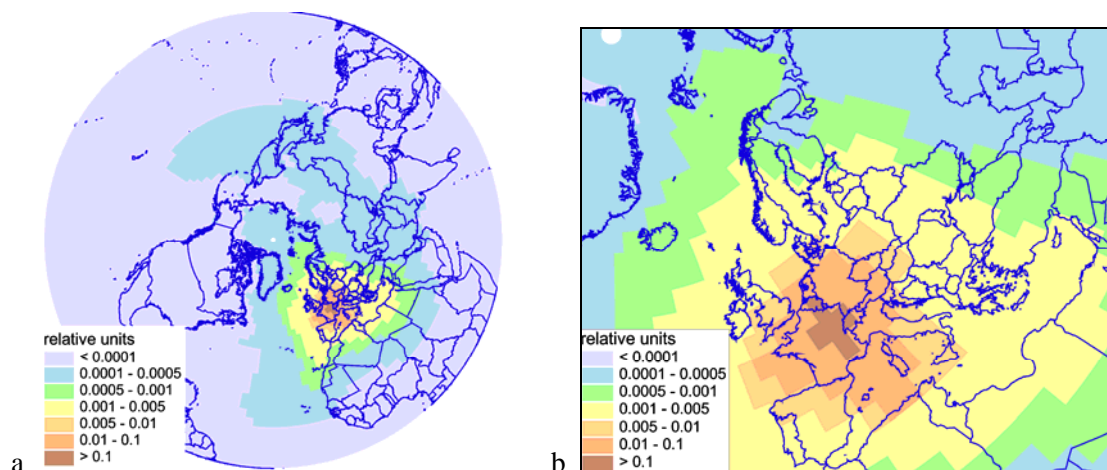
As seen from the calculated balance, the removal of this PCN congener from the atmosphere is determined approximately to the same extent by degradation and deposition processes. Within a year 54% of PCN-47 are degraded in the atmosphere and 46% are deposited to the different types of underlying surface. Here, the most part of deposited pollutant (36%) is accumulated in soil and the rest (10%) is in seawater. So, the character of the presented balance can be explained not only by the physical-chemical properties of the considered substance (degradation rate constants, subcooled liquid-vapour pressure values and Henry's law constants) but also by the type of underlying surfaces and some meteorological parameters.

The considered congener of tetra-CN<sub>s</sub> exists in the atmosphere both in the gas and particulate phases with considerable predominance of the gaseous phase. Its degradation in the atmosphere is governed by the second-order rate constant equal to  $9.11 \cdot 10^{-13} \text{ cm}^3/\text{molec} \cdot \text{s}$  estimated for its gas-phase interaction with OH radical [Howard and Meylan, 1997]. Taking into account the degradation process only, the atmospheric half-life of PCN-47 obtained with the use of average value of OH radical spatial distribution used in the model ( $8.8 \cdot 10^5 \text{ molecule}/\text{cm}^3$ ) is 10 days.

The residence time of PCN-47 in the atmosphere ( $T_{1/2}^{\text{air}}$ ) estimated on the basis of model calculations of its atmospheric transport is amounted to 7 days. So, for this pollutant the numerical characteristic of LRTP obtained by modelling meets the existing criterion for POPs (atmospheric half-life is greater than two days).

## 1.2. Spatial distribution of pollution from conventional emission source

Additional information on LRTP of the considered chemical is provided by the spatial distribution of PCN air pollution estimated by modelling on the basis of its atmospheric transport from the conventional point emission source and atmospheric balance. In Fig 2a,b concentration fields of PCN-47 in the Northern Hemisphere and EMEP domain are given. For convenience, air concentrations are presented in the relative units i.e. as ratios of the concentration calculated in the particular point to the concentration near a source.



**Fig. 2.** Spatial distribution of PCN-47 concentrations in the above-ground air in the Northern Hemisphere and in the EMEP domain

According to the model assessment, the area of air pollution with PCN-47 from the conventional point source, where air concentration is 1000 times lower than that near the source, is located over the most part of Europe, includes Mediterranean Sea, and some part of the Atlantic ocean and reaches the Arctic region and northern Africa. The levels of air concentrations over most European countries vary from 0.001 to 0.1 of the basic value.

The model assessment demonstrates that PCNs emitted from a conventional European source of such intensity are capable to cause air pollution over the considerable areas including remote regions located far from the source. Available data on measurements of PCN air concentrations in different region of the Northern Hemisphere also testify that this group of pollutants is ubiquitous. Measured air concentrations of PCNs available from the literature along with data on congener profiles in the screened samples are presented in Table 1.

According to the data presented, the range of measured PCN air concentrations is wide varying from 0.8 (Dunai Island, Russia) to 175  $\mu\text{g}/\text{m}^3$  (Chicago, USA). Values of total toxicity given in  $\Sigma\text{TEQ}$  do not exceed 3.6  $\text{fg}/\text{m}^3$ . Homological groups of tri- and tetra-CNs are detected in prevalent quantities in all analysed air samples in comparison with other CN groups.



**Table 2. Measured air concentrations of PCNs**

Sampling site	Sampling date	Concentrations $\Sigma$ PCN, $\mu\text{g}/\text{m}^3$		Congener profile, %	References
		$\mu\text{g}/\text{m}^3$	$\Sigma$ TEQ, $\text{fg}/\text{m}^3$		
<b>Germany</b>					
Ausburg	VI. 1992-II. 1993	60		Tri-CNs – 76.5; Tetra-CNs – 19.3; Penta-CNs – 2.9.	<i>Dörr et al., 1996</i>
Background station near Ausburg	VI. 1992-II. 1993	24		Tri-CNs – 76.4; Tetra-CNs – 17.0; Penta-CNs – 4.5.	
<b>UK</b>					
Lancaster (Hazellrig)	1994	66			<i>Harner et al., 2000</i>
Lancaster	1995	152	3.6	Tri-CNs – 44; Tetra-CNs – 51.5; Penta-CNs – 3.4.	<i>Lee et al., 2000</i>
Hazellrig	1998-1999	38.5			<i>Harner et al., 2000</i>
High Muffles	1998-1999	26.5			
Stoke Ferry	1998-1999	31			
Manchester	1998-1999	<u>138-160</u> 149			
<b>Sweden</b>					
Hoburgen	1990-1991	5.07		Tri-CNs	<i>Egebäck et al., 2004</i>
Ammarnäs	1990-1991	1.55			
<b>USA</b>					
Chicago, IL	II–III, 1995	<u>24-175</u> 68		PCN-24 – 40; PCN-33 – 10; PCN- 38 - >9.	<i>Harner and Bidleman, 1997</i>
<b>Canada</b>					
Lake Superior	VIII 1996	3.25*			<i>Helm et al., 2003</i>
	V 1997	1.82*			
Lake Ontario	VII, IX 1998	4.27*			
	VI 2000	12.3		Tri-CNs – 54.4; Tetra-CNs – 36.3; Penta-CNs – 8.2.	
Cornwall	II 1999	6.38		Tri-CNs – 46.4; Tetra-CNs – 41.8; Penta-CNs – 9.7.	
Downaview, near Toronto	III, 1995	<u>12-22</u> 17			<i>Harner and Bidleman, 1997</i>
Totonto, UT	2000-2001	<u>31-78</u> 51.1	<u>0.5-2.2</u> 1.4	Tri-CNs – 32; Tetra-CNs – 49; Penta-CNs – 17.	<i>Helm and Bidleman, 2003</i>
Toronto, MSC	2000-2001	<u>7-84</u> 28	<u>0.08-0.53</u> 0.30	Tri-CNs – 47; Tetra-CNs – 41; Penta-CNs – 9.	
<b>Polar regions</b>					
Barents Sea	1996	40	0.99	Tri-CNs – 42; Tetra-CNs – 47; Penta-CNs – 8.	<i>Harner et al., 1998</i>
Norwegian Sea	1996	7.1	0.36	Tri-CNs – 46; Tetra-CNs – 39; Penta-CNs – 10.	
E. Arctic Ocean	1996	12	0.55	Tri-CNs – 48; Tetra-CNs – 37; Penta-CNs – 9.	
Alert, Canada	1993-1994	3.5	0.076	Tri-CNs – 69.5; Tetra-CNs – 19.8; Penta-CNs – 2.7.	
Dunai Island, Russia	1993	0.8	0.092	Tri-CNs – 54.2; Tetra-CNs – 37.6; Penta-CNs – 5.3.	

\* - summa tetra- hexa-CNs; Tri-CNs – tetra-chlorinated naphthalenes; Tetra-CNs - tetra-chlorinated naphthalenes; Penta-CNs - penta-chlorinated naphthalenes; Hexa-CNs - hexa-chlorinated naphthalenes.

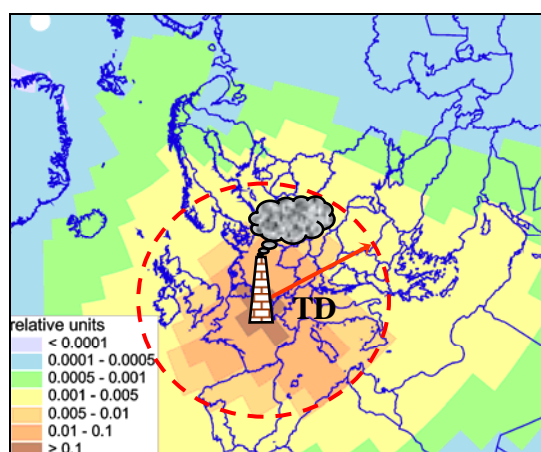
### 1.3. Transport Distance

At present several model approaches to evaluation of LRTP of a pollutant by means of different numerical characteristics have been developed and introduced in [Scheringer and Berg, 1994; Scheringer, 1996; Bennett et al., 1998; van Pul et al., 1998; Wania, 1998; Rodan et al., 1999; Beyer et al., 2000; Beyer et al., 2001; Beyer and Matthies, 2001; Leip and Lammel, 2004, etc]. For example such characteristics are spatial range, spatial scale, transport distance, characteristic travel distance, travelling distance, and so on. In this assessment in addition to the atmospheric residence time of PCN-47, another characteristic demonstrating LRTP of the considered substance is provided by the model estimate of its *Transport Distance* (TD). Numerical values of TD are defined with the help of Eq. 1 as the average distance from the source at which annual mean atmospheric concentration of a chemical in question drops 1000 times compared with the concentration near the point source (as an example See Fig.3):

$$TD_{0.001} = \sqrt{\frac{S_{0.001}}{\pi}} \quad (1)$$

where  $S_{0.001}$  is the area covered by air concentrations dropped less than 1000 times.

It should be noted that such an approach is similar to that suggested in [Rodan et al., 1999].



**Fig. 3.** Definition of the transport distance

The value of *TD* depends on all of the processes removing the pollutant from the atmosphere such as deposition to the underlying surface (land, sea) and atmospheric degradation. It was found that for PCN-47 processes of degradation and depositions to different types of underlying surfaces contribute almost equally to its removal from the atmosphere and produce equal effect on the calculated value of *TD*. The calculated value of *TD* for PCN-47 is amounted to 2271 km. Both characteristics of LRTP obtained for PCN-47 with the help of model calculations are presented in Table 2.

**Table 2.** Characteristics of LRTP (*Half-life in air<sub>calc</sub>* and *Transport Distance*) calculated for PCN-47

Substance	$T_{1/2}^{air}$ , days	<i>TD</i> , km
PCN-47	7	2271

The presented numerical characteristics of LRTP for PCN-47 fully meet the LRTP criteria of Executive Body Decision 1998/2.

## 2. PERSISTENCE

The behaviour of a substance in the environment to a large extent is determined by its persistence not only in the atmosphere but also in other environmental media. Its redistribution between air and soil, seawater, sediment, vegetation etc is important for its ability to be accumulated in the food chain. In this process the main characteristic is its half-life in the media under consideration.

In compliance with the Executive Body Decision 1998/2 the persistence of “new substances” in terms of their possible inclusion into the Protocol on POPs is demonstrated by indicative numerical values of their half-life in water, which should be greater than two months, or half-life in soil, which should be greater than six months, or half-life in sediments, which should be greater than six months also. In addition to these parameters characterizing the persistence for particular media, multimedia model calculations allow estimating complementary characteristics of persistence in the whole environment - overall residence time or overall environmental persistence [Scheringer, 1996; Webster *et al.*, 1998; Gouin *et al.*, 2000, etc]. In this assessment such characteristic as *Half-life in the environment* ( $T_{1/2}^{env}$ ) is estimated for the considered pollutant on the basis of the model calculations of its atmospheric transport taking into account deposition processes, degradation and gaseous exchange between main environmental media.

The model assessment of persistence in the environment for PCN-47 is demonstrated by the numerical value of  $T_{1/2}^{env}$  calculated with the help of Eq.2 as an inverse value of weighted mean of degradation rate constants  $k_j$  in the environmental media (atmosphere, soil, seawater, vegetation, sediments) with weights being the fractions  $f_j$  of a pollutant accumulated in  $j$ -th medium:

$$T_{1/2}^{env} = \ln 2 / \sum k_j \cdot f_j \quad (2)$$

Here fractions  $f_j$  are evaluated on the basis of the model calculations.

Thus, the value of *Half-life in the environment* is affected by the distribution of the total environmental content of PCN-47 between main environmental media (air, soil, water, sediment and vegetation) and the values of its half-life in each particular medium due to degradation process.

The distribution of PCN total content in the environment between main environmental media (annual media balance) and relative fractions of the pollutant degraded in each media during a year (annual degradation balance) were obtained on the basis of simulations for one-year period. It should be noted that seawater includes pollutant content in sediments, and only degradation in forest litter is considered as degradation in vegetation. The annual media balance of PCN-47 in comparison with its annual degradation balance is shown in Fig.4.

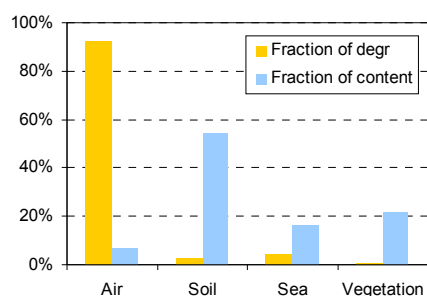


Fig. 4.. Annual degradation and media balances for PCN-47

Degradation of this pollutant in the atmosphere is substantially more rapid than that in other environmental media coming to approximately 92% of PCN-47 amount degraded in the environment by the end of a year. Relative fractions of the pollutant degraded in each other media are the following: approximately 4% for seawater; 3% for soil and 0.5 for vegetation. At that, due to deposition processes within a one-year period more than a half of overall PCN-47 content in the environment (~55%) is accumulated in soil and only 7% remain in the atmosphere. Its content in seawater and vegetation equals 16 and 22%, respectively. Soil is appeared to be the main medium accumulating this pollutant. The distribution of PCNs in the environment and their levels in different environmental compartments can be illustrated with the help of monitoring data given in Annex A.

The value of *Half-life in the environment* for PCN-47 calculated on the basis of annual media and degradation balances totals to 95 days or approximately 3.2 months. The calculated estimate of  $T_{1/2}^{env}$  together with values of half-life in the particular environmental media used for modelling [HSDB, 2002] is presented in Table 3.

**Table 3.** Characteristics of Persistence (*Half-life in environment*) and half-life of PCN-47 in different environmental media used for modelling of atmospheric transport

Substance	$T_{1/2}^{env}$ , months	Half-life, months		
		air	water	soil
PCN-47	3.2	0.3	12	57

According to the calculated value of *Half-life in the environment*, persistence of PCN-47 in the environment can be characterised as moderate. At that the obtained value of  $T_{1/2}^{env}$  is considerably lower than those of half-life due to degradation process in soil and seawater and higher than that for degradation in the atmosphere only. Due to relatively high ability of PCN-47 to accumulate in soil, this pollutant may course long-term adverse affect through this medium.

### 3. BENCHMARK APPROACH

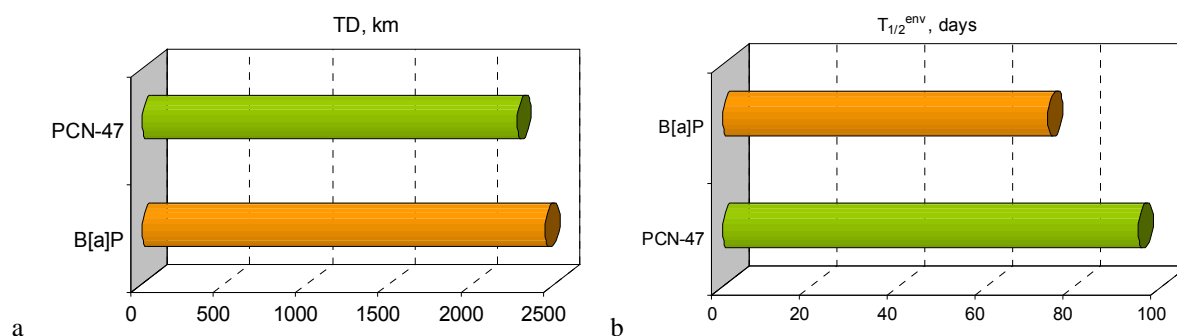
Since the numerical values of  $T_{1/2}^{air}$  and  $T_{1/2}^{env}$  of particular chemicals are model dependent, one of the possible ways to diminish uncertainties in evaluating new substances proposed by Scheringer [1997] and Beyer *et al.* [2000] and discussed at the OECD/UNEP Workshop on the Use of Multimedia Models for the Estimation of Environmental Persistence and Long-Range Transport (Ottawa, Canada, 2001) was to use a “benchmark” approach. This approach suggests that model results on LRTP and persistence are used to compare the pollutants under study with some adequately studied “benchmark substance” with known values of the considered parameters.

This procedure enables assessment of “new substance”, by considering their ranking in terms of persistence or LRTP among the well-known benchmark chemicals. Examples of chemicals ranking and classification approach are described by Matthies *et al.* [1999], and Bennett *et al.* [2001]. Relative approach may also be applicable when the desired outcome is the screening of a large set of existing chemicals, to establish priority classes of substances for further assessment or action [ENV/JM/MONO(2004)5, 2004].

The comparison of calculated characteristics of LRTP and persistence for PCN-47 against those obtained for a benchmark pollutant is presented in this subsection. Benzo[a]pyrene (B[a]P) is used as a benchmark substance in this assessment. Characteristics of its behaviour in the environment are

well studied and clearly meet UN ECE criteria for POPs. It is already included in the Protocol on POPs and is considered as pollutant of regional concern. All calculations were performed for one-year period from a conventional point source with one and the same location in Europe and one and the same emissions intensity.

The considered PCN-47 and B[a]P have been ranked in ascending order according to their values of *Transport Distance* (Fig. 5a) and *Half-life in the environment* (Fig. 5b).



**Fig. 5.** *Transport distance and Half-life in the environment* calculated for PCN-47 and B[a]P

According to the model calculations of *TD*, LRTP of the considered congener of tetra-CNs is close to that of B[a]P, though slightly lower. Persistence of PCN-47 in the environment is somewhat higher than that of B[a]P (95 days compared to 74 days for B[a]P).

Thus, according to the results on ranking the considered substances, the numerical characteristics of LRTP and persistence of PCN-47 are comparable with those of the adequately studied “benchmark” pollutant already included into the Protocol on POPs.

#### **4. CHARACTERISTICS OF PCN LRTP AND PERSISTENCE IN RELATION TO THE INDICATIVE CRITERIA OUTLINED IN EXECUTIVE BODY DECISION 1998/2**

As it was stated above this model assessment was carried out for PCN-47 chosen as a representative of all possible congeners of PCNs (see Annex A). This assumption was made since the considered congener belongs to the homological group of tetra-CNs, which are detected in the most part of emission source samples and samples taken from remote sites. In this connection, physical-chemical properties of tetra-CNs presented in [van de Plassche and Schwegler, 2002] are given in Table 5 in relation to the LRTP and persistence criteria outlined in the Executive Body Decision 1998/2 with additions of the MSCE-POP model estimates. Data on physical-chemical properties of PCN-47 available in [van de Plassche and Schwegler, 2002] and used in the model calculations are given in the Annex B (Tables B1 and B2).

**Table 5.** Comparison of LRTP and persistence of tetra-CN and criteria of Executive Body Decision 1998/2 based on data [van de Plassche and Schwegler, 2002] and with additions of MSCE-POP model estimates

Criterion	Criterion values	Meets the criterion (Yes/No)	Characteristics of TetraCN	Remarks
<i>Potential for Long-Range Transboundary Atmospheric Transport</i>				
Vapour pressure, Pa	< 1000	Yes	0.048 at 25 °C	Presented in <i>van de Plassche and Schwegler, 2002</i> $T_{1/2}^{air}$ calculated by MSC-E
Half-life in air, days	>2	Yes	18	
Half-life in air <sub>calc.</sub> , days		Yes	7	
<i>Persistence</i>				
Half-life in water, months	> 2	Yes		Presented in <i>van de Plassche and Schwegler, 2002</i>
Half-life in soil, months	>6	Yes		
Half-life in sediment, months	>6	Yes		
Half-life in the environment, months	-	-	3.2	$T_{1/2}^{env}$ calculated by MSC-E

The results of the model assessment demonstrate the considerable long-range atmospheric transport potential and persistence of PCN-47 in the environment. This conclusion is also confirmed by the comparison of calculated numerical characteristics of LRTP and persistence of dicofol against those obtained for typical POP of regional concern – B[a]P. However, since in this model assessment the behaviour of PCNs in the environment was studied on the example of one selected homological group, further detailed analysis of model results on LRTP and persistence of other groups is required.

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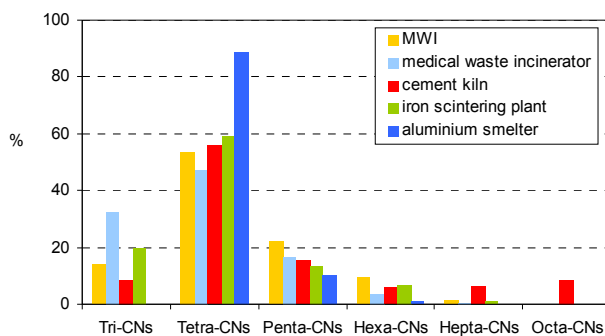
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## CONGENER PROFILES AND LEVELS OF PCNS MEASURED IN EMISSION AND ENVIRONMENTAL SAMPLES

The model assessment of LRTP and persistence of PCNs is carried out for PCN-47. This congener was selected as a representative of the homological group of tetra-chlorinated naphthalenes, which is prevalent in PCN congener profiles of most types of environmental and source related samples analysed. The choice of the considered congener is based on the available data on PCN congener profiles, patterns and levels detected in different types of emission sources and concentrations in the main environmental media. The analysed data are presented briefly in this Annex.

### *Emission sources of PCNs in the environment*

Waste incineration along with other thermal processes is one of the most important pathways of PCN entry to the environment. Content and congener profiles of PCNs identified in emission samples collected from different types of waste incinerators have been investigated within several studies [Sakai *et al.*, 1996; Schneider *et al.*, 1998; Abad *et al.*, 1999]. Homologue mass distribution of the considered pollutants in fly ash of municipal solid waste incinerators, cement kilns, medical waste incinerator and iron sintering plant was compared in the study of Helm and Bidleman [2003]. PCN congener profile in the flue gas of aluminium smelter plant was identified by Aitolla *et al.* [1996]. Comparison of homological profiles of PCNs detected in samples collected from different emission sources is presented in Fig. A1.



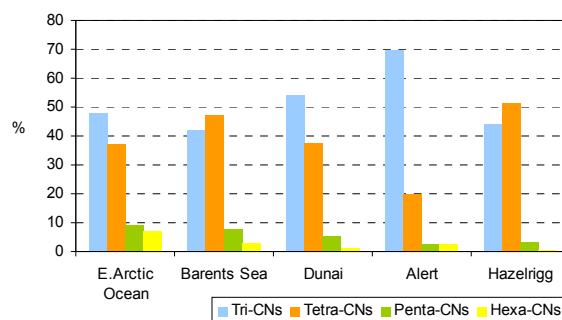
**Fig.A1.** Comparison of homological profiles of PCNs identified in samples collected from different emission sources

According to the data presented, the contribution of homological group of tetra-CNs to the total PCN emissions from different types of thermal sources is the most substantial as compared with other groups. Besides, it was found that in the most emission samples analyzed considerable variations in PCN concentrations were observed. In particular, PCN concentration in the flue gases of aluminium smelter amounted to 2981 ng/m<sup>3</sup>, whereas in the flue gases of MWI it was in the range from 1 to 21 ng/m<sup>3</sup>. The highest level of these pollutants was measured in the fly ash from medical waste incinerators up to 5439 ng/m<sup>3</sup>.

Pyrolysis of polyvinylchloride (pvc) is reported to be another important emission source of PCNs [HSDB, 2002]. During this process tetra-CN's are formed in the prevalent quantities (94.5-104 mkg/g) in comparison with other homological groups.

### ***Air concentrations***

Air concentration levels of PCNs have been monitored in different regions including those located far from emission sources such as the Arctic region (see Table 2 in Section 1.2). PCN congener profiles detected in air samples taken in different remote and background regions are demonstrated in Fig. A2.



***Fig. A2. Congener profile of PCNs in the air concentrations***

It can be noted that for all considered sampling sites the groups of lighter congeners – tri- and tetra-CN's are found to be detected in the larger quantities than other groups. Several studies of PCN air pollution in the Central Europe and in the Great Lakes region demonstrated the similar homologue distribution.

### ***Soil concentrations***

The distribution of PCNs in soil samples collected at different region of the Northern Hemisphere can be illustrated with the help of monitoring data available in the literature (see Table A1).

**Table A1. PCN soil concentrations**

Sampling site	Sampling date	Soil concentrations of $\Sigma$ PCN		Congener profile, %	References
		ng/g	$\Sigma$ TEQ, pg/g dw		
<b>UK</b>					
Rothamsted station, 42 km north of London (archived soil)	1986	0.32	0.008	Tri-CNs – 44.6 Tetra-CNs – 42.5 Penta-CNs – 3.1 Hexa-CNs – 2.3 Hepta-CNs – 1.5	<i>Meijer et al., 2001</i>
Ludington 30 km south of Birmingham (archived soil)	1990	0.42	0.012		
Contemporary soils, southwest of the U.K collected at several sites across the U.K	1993	0.35			<i>Harner et al., 1999</i>
<b>Germany, Bayreuth, northern Bavaria</b>					
urban area	Before 2003	Nd – 15, 4			<i>Krauss and Wilcke, 2003</i>
industrial		0.67 – 15.0		Tri-CNs – 4.5 Tetra-CNs – 28.4 Penta-CNs – 38.2 Hexa-CNs – 23.2 Hepta-CNs – 4.7	
agricultural		n.d – 0.51			
rural sites		Nd – 0.82		Tri-CNs – 5.5 Tetra-CNs – 30.6 Penta-CNs – 30.9 Hexa-CNs – 25.5 Hepta-CNs – 7.5	
<b>Spain, Tarragona County</b>					
Chemical industries	2002	0.12		Tetra-CNs – 34.4 Penta-CNs – 28.2 Hexa-CNs – 23.2 Hepta-CNs – 10.2 *Cl <sub>8</sub> N – 4.1	<i>Schumacher et al., 2004</i>
Oil refinery and petrochemical industries		0.07		Tetra-CNs – 16.2 Penta-CNs – 22.5 Hexa-CNs – 10.8 * Hepta-CNs – 4.1 * Octa-CNs – 4.1	
Residential (urban)		0.18		Tetra-CNs – 34.6 Penta-CNs – 42.4 Hexa-CNs – 15.3 Hepta-CNs – 4.9 * Octa-CNs – 2.8	
unpolluted		0.03		Tetra-CNs – 31.9 Penta-CNs – 21.8 * Hexa-CNs – 15.8 * Hepta-CNs – 15.8 * Octa-CNs – 15.8	
<b>USA, Brunswick, GA</b>					
southern coastal Georgia near chlor-alkali plant	II, 1996	17900	5330	Tri-CNs – 0.5 Tetra-CNs – 3.6 Penta-CNs – 12.4 Hexa-CNs – 32.4 Hepta-CNs – 39.8 Octa-CNs – 11.3	<i>Kannan et al., 1998</i>

\* Hepta-CNs – 4.1 - sum PCN was calculated assuming that when in a group of homologues the sum was below the limit of detection (10 ng/g), this sum was equal to one-half of this limit;

Tri-CNs – tetra-chlorinated naphthalenes;

Hexa-CNs - hexa-chlorinated naphthalenes;

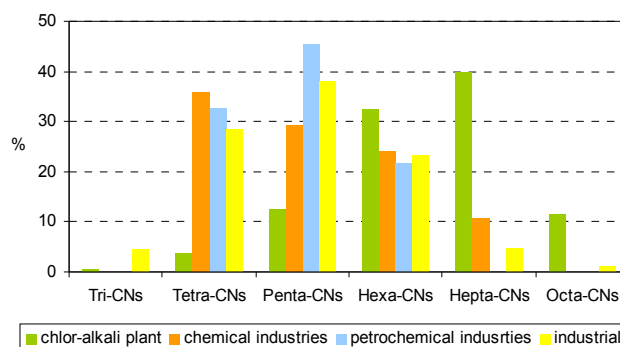
Tetra-CNs - tetra-chlorinated naphthalenes;

Hepta-CNs - hepta-chlorinated naphthalenes;

Penta-CNs - penta-chlorinated naphthalenes;

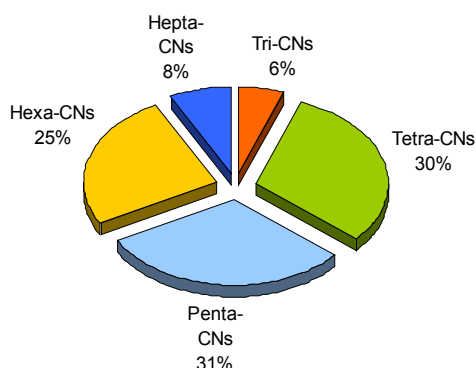
Octa-CNs - octa-chlorinated naphthalenes.

The influence of industrial sources on homologue distribution of PCNs in soils is shown in Fig.A3. The data on soil pollution measured near by different productions were taken for this diagram from the following studies: chlor-alkali plant - *Kannan et al.* [1998]; chemical industry and petrochemical industry - *Schumacher et al.* [2004]; industrial - *Krauss and Wilcke* [2003]. In soil samples collected near industrial sources of northern Bavaria, Germany tetra- and penta- CNs are prevalent among other homological groups.



**Fig. A3.** Homological profile of PCNs in industrial soils

Main features of PCN distribution in rural soils of Bavaria have been investigated in the study of *Krauss and Wilcke* [2003] (see Fig. A4). Here, tetra- and penta-CNs are detected also in the larger quantities than other groups.



**Fig. A4.** Homological profile of PCNs in soils of rural area in northern Bavaria

### **Water concentrations**

Available data on monitoring of water pollution by PCNs are very scarce in the literature. In particular, there are data on levels of water concentrations in the lake Ontario, Canada [*Helm et al.*, 2003] and in a lake and river polluted by PCBs in Scandinavia [*Järnberg et al.*, 1997].

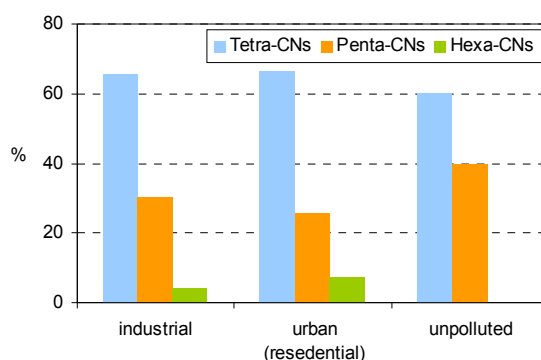
In the samples collected from the surface water of the lake Ontario the analysis was made for the high volume of water (100 L) and for the dissolved phase of pollutants. At that, only tri- and tetra- CNs were identified there. Observed levels of water concentrations were within the range from 16.35 to 24.48 pg/L. In all samples concentrations of tri-CN homological group were from 1.7 to 3.5 times higher than that of tetra-CNs.

Measured levels of water concentrations in the river Emån and the lake Järnsjön, polluted with PCBs, considerably exceed those in the lake Ontario amounting to 890 pg/L. Tetra-, penta-, hexa- and hepta-homologous group were detected in the analysed samples. In this region contribution of tetra-CNs to the total content of PCNs was dominated and come to 1.6 times.

### *Concentration in vegetation*

Limited number of monitoring data on PCN concentrations in vegetation was found in the literature. Total PCN concentrations in grasses sampled in semi-rural field station site in the northwest of England were measured in the study of *Harner et al.* [1999]. Total concentration of PCNs in this region amounted to 2.12 ng/g of dry weight. This study revealed also that the groups of lighter congeners – tri- and tetra-CNs prevailed over other groups.

The concentration of PCNs have been determined in wild chard samples collected in an area of Tarragona County (Catalonia, Spain) with an important number of chemical and petrochemical industries [*Schumacher et al.*, 2004]. Samples were also collected in urban/residential zones, as well as in presumably unpolluted sites. There were insignificant differences among collecting zones in the levels of PCNs found in chard. PCN concentration detected at the industrial sampling sites was equal to 214 ng/kg of dry weight; at the urban sites – 172 ng/kg of dry weight, and at the unpolluted sites – 146 ng/kg of dry weight. Homologue distribution of PCNs in samples of vegetation presented in [*Schumacher et al.*, 2004] is shown in Fig. A5.



**Fig. A5.** Homologue distribution of PCNs in vegetation samples collected in Catalonia, Spain.

As seen from the data presented, in all analyzed samples of wild chard the group of tetra-CNs was found to be in predominant quantities as compared with other groups. Its fraction amounted to more than a half (not less than 60%) of the total PCN content measured in all the samples.

Thus, for the sake of model assessment of LRTP and persistence for PCNs, homologous group of tetra-CNs, which prevails over other groups in the most part of source-related samples and samples taken from main environmental media, was chosen on the basis of available measurement data on PCN congener profiles. PCN-47 was selected among other tetra-CNs because of availability of all physical-chemical properties and degradation rates required for modelling.

## PHYSICAL-CHEMICAL PROPERTIES OF POLYCHLORINATED NAPHTHALENES USED FOR MODELING

The key physical-chemical properties and degradation rates of tetra-CN<sub>s</sub> presented in [van Plassche and Schwegler, 2002] are shown in Table B1.

**Table B1.** Physical-chemical properties of tetra-CN<sub>s</sub> presented in [Plassche and Schwegler, 2002]

Physical chemical properties	Numerical values
<b>Vapour pressure, Pa</b>	0.048 at 25 °C
Solubility in water, mg/L	0.004
Henry's Law constant, Pa·m <sup>3</sup> /mol	16.06
Octanol-water partition coefficient (log <i>K<sub>OW</sub></i> )	6.19
<b>Half-life, days</b>	
Air	18
Water	
Soil	
Sediment	

References: Crookes and Howe, 1993; Syracuse in HSDB, 2000

The full set of physical-chemical properties and degradation rates of PCN-47 selected for the model parameterisation on the basis of data available in literature is presented in Table B2. Temperature dependences of some physical-chemical characteristics (Henry's law constant, subcooled liquid-vapour pressure, octanol-air partition coefficient) are given at reference temperature equal to 283.15 K.

**Table B2.** Physical-chemical properties of PCN-47 used for modelling

Physical-chemical properties	Numerical values	References
Henry's law constant for fresh and sea water at 10 °C, Pa·m <sup>3</sup> /mol	2.91	Estimated on the basis of temperature dependence of $K_{OA}$ given in <i>Harner and Bidleman</i> , 1998
Coefficient of Henry's constant temperature dependences, K	9617	
Subcooled liquid-vapour pressure at 10 °C, Pa	$5.88 \cdot 10^{-3}$	<i>Lei et al.</i> , 1999
Coefficient of subcooled liquid – vapour pressure temperature dependences, K	8666	
Rate constant of reaction with OH radical in air, cm <sup>3</sup> /(molec·sec)	$9.11 \cdot 10^{-13}$	<i>Howard and Meylan</i> , 1997
Degradation rate constant in air, s <sup>-1</sup>	$8.02 \cdot 10^{-7}$	Calculated with the use of average value of OH-spatial distribution used in the model: [OH] = $8.8 \cdot 10^5$ molec/cm <sup>3</sup>
Half-life in air, days	10	
Degradation rate constant in water, s <sup>-1</sup>	$2.19 \cdot 10^{-8}$	Estimated
Half-life in water, days	366	<i>HSDB</i> , 2001
Degradation rate constant in soil, s <sup>-1</sup>	$4.72 \cdot 10^{-9}$	Estimated
Half-life in soil, months	1700	<i>Hazardous Substances Databank - HSDB</i> , 2002
Molar volume, cm <sup>3</sup> /mol	228	<i>Lei et al.</i> , 1999
«Octanol-water» partition coefficient at 25 °C	$8.65 \cdot 10^5$	Estimated with the use of $K_{OA}$ taken from <i>Harner and Bidleman</i> , 1998
«Octanol-air» partition coefficient at 10 °C	$7.00 \cdot 10^8$	<i>Harner and Bidleman</i> , 1998
Coefficient of $K_{OA}$ temperature dependences, K	9257	
Molecular diffusion coefficients, m <sup>2</sup> /s:		Calculated with the help of equations from <i>Swarzenbach et al.</i> , 1993
in water	$6.15 \cdot 10^{-10}$	
in air	$5.37 \cdot 10^{-6}$	
“Organic carbon-water” partition coefficient, m <sup>3</sup> /kg	354	Calculated with the help of relationship between $K_{OC}$ and $K_{OW}$ given in <i>Karickhoff</i> , 1981