EMEP CONTRIBUTION TO THE PREPARATORY WORK FOR THE REVIEW OF THE CLRTAP PROTOCOL ON POPS

NEW SUBSTANCES:

Model assessment of potential for long-range transboundary atmospheric transport and persistence of Pentachlorophenol (PCP)

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CONTENTS

INTRODUCTION

Pentachlorophenol (PCP) is a synthetic substance that was first produced in the 1930s. It is marketed under the trade names Santophen, Pentachlorol, Chlorophen, Chlon, Dowicide 7, Pentacon, Penwar, Sinituho and Penta among others. In the past, it has been used as a herbicide, insecticide, fungicide, algaecide, disinfectant and as an ingredient in antifouling paint. Some applications were in agricultural seeds (for nonfood uses), leather, masonry, wood preservation, cooling tower water, rope and paper mill system. PCP was widely used also not only by itself but also in the form of water-soluble salts - sodium pentachlorophenate (NaPCP) and pentachlorophenyl laurate (PCPL).

Evaluation of PCP production volumes was performed in the beginning of 80th. At this moment annual production in North America and Europe was 50 – 60 thousands tons per year. In China PCP production amounted to about 5 thousand tons per year [*Borysiewicz,* 2008].

The marketing and use of PCP and its compounds was prohibited in the EU in 1991. PCP, NaPCP and PCPL may be used in the remedial treatment of timber and as a surface biocide for masonry. Production of PCP and NaPCP ceased in the EU in 1992. After that these chemicals have been imported to the EU from USA. The main use of PCP today in the OSPAR regions is the production of PCLP [*Pentachlorophenol. Hazardous Substances Series. OSPAR,* 2001]. PCPL is used in the preservation of textiles, which are subject to attack by fungy and bacteria during storage and use. Production of PCPL ceased in European Union in 2000 since according to Commission Directive 1999/51/EC use of PCP and its compounds is not permitted as a synthesizing and/or processing agent in industrial processes from 1 September 2000 [*Borysiewicz,* 2008].

PCP is a potential candidate for the inclusion into the Protocol on POPs to the Convention on Long-Range Transboundary Air Pollution (Twenty-sixth session of the Executive Body held in Geneva in December 2008).

This Technical Note presents additional information for the evaluation of PCP as a potential new POP in accordance with the two criteria: potential for long-range transboundary atmospheric transport (LRTP) and persistence. The work is carried out by the request of the Executive Body for CLRTAP

For the evaluation of LRTP and persistence of pollutants, MSCE-POP multicompartment hemispheric transport model is used. Detailed information on the structure of the model and parameterisation of the media processes can be found in the MSC-E reports [*Gusev et al.,* 2005] and on the Internet (http://www.msceast.org).

To estimate the considered parameters for PCP, the model calculation of its atmospheric transport from a conventional point emission source located in Europe 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.

Presented information is divided into four parts.

1. To evaluate **LRTP** of PCP, two numerical characteristics are calculated. The first one is residence time in the atmosphere (**Half-life in air$_{calc}$** ($T_{1/2}{}^{air}$)) 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 PCP is provided by the spatial distribution of air pollution caused by the considered conventional point emission source.

2. **Persistence** in the environment is evaluated by *Half-life in the environment* ($T_{1/2}^{env}$) estimated for PCP 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.

3. The values of *TD* and $T_{1/2}^{env}$, calculated by the model depend on model characteristics (such as resolution, spatial coverage, etc.). To exclude model peculiarities in evaluating LRTP and persistence of PCP, a comparison of their numerical values against those obtained for an adequately studied "**benchmark substance**" is presented.

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

Since measurement data in remote regions are mentioned among the criteria for recognizing a substance as a POP, a short review of existing data on levels of PCP measured in environmental samples is presented in Annex A to the report. Annex B includes the summary of PCP physical-chemical properties used for modelling.

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.

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$_{calc}$* ($T_{1/2}^{air}$)) 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, which are, in turn, affected by other environmental processes, e. g. gas/particle partitioning. Advantages of modelling approach are contained in possibility to distinguish the most important processes affecting LRTP of a particular considered pollutant in the atmosphere taking into account "real" environmental conditions. 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 Section contains the main results on evaluation of LRTP criterion for PCP with the help of above-mentioned characteristics obtained on the basis of the hemispheric MSCE-POP model calculations.

1.1. Residence time in the atmosphere

To estimate the residence time in the atmosphere, the model calculation of atmospheric transport of PCP 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 PCP to the atmosphere are assumed to be 1 tonne per year from a conventional point emission source located in Europe (5°E; 47.5°N). On the basis of this calculation annual atmospheric balance of the removal of PCP from the atmosphere is estimated (see Fig.1).

According to the model assessment, removal from the atmosphere is mainly attributed to dry deposition over land (about 65% of total removal) and degradation (about 30% of total removal) processes. The character of the presented balance is governed 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.

Calculated value of residence time in the atmosphere (Half-life in air$_{calc}$ ($T_{1/2}^{air}$)) for PCP occurs to be of about **7.4 days**.
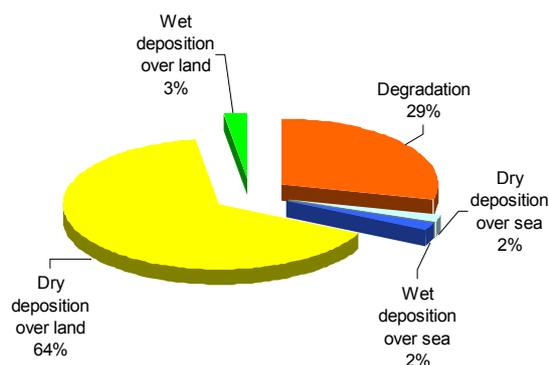

Fig. 1. *Calculated annual balance of PCP removal from the atmosphere*

1.2. Spatial distribution of pollution from conventional emission source

Additional information on LRTP of PCP is provided by the spatial distribution of its air pollution obtained on the basis of simulation of its atmospheric transport from the considered conventional point emission source. In Fig. 2 air concentration fields of PCP in the Northern Hemisphere and EMEP domain are given. For convenience, 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.
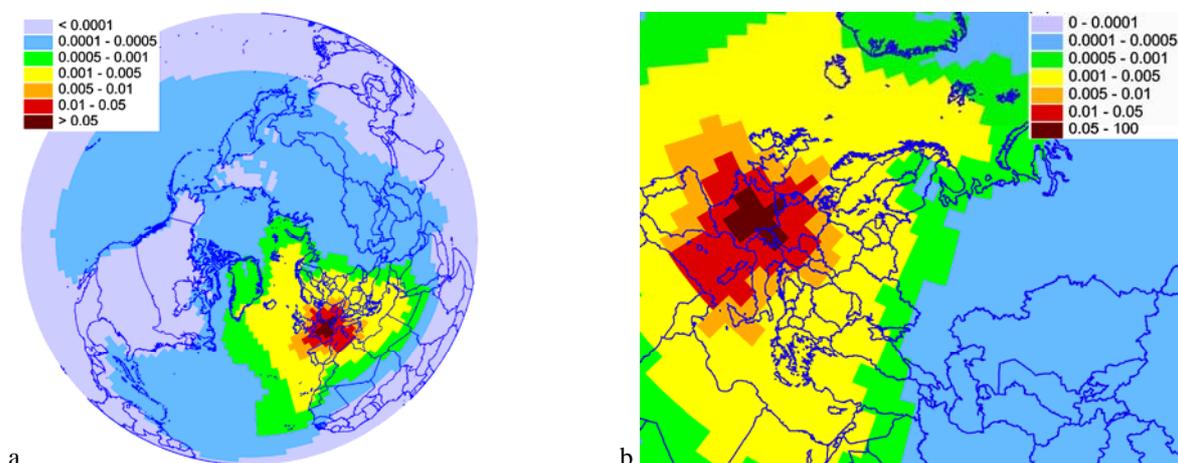

Fig. 2. *Spatial distribution of pentachlorophenol concentrations in the above-ground air in the Northern Hemisphere (a) and in the EMEP domain (b), relative units*

With a conventional source of emissions located in Europe, the area of atmospheric air concentration of PCP, which is 1000 times lower than the concentration near the source, is located over almost all Europe, including Mediterranean Sea and reaching northern Africa and middle-Atlantic. Considering the influence of the emission source on the EMEP domain (see Fig.2b) shows that the most intensive air pollution by PCP is characteristic of territories of France and its neighboring countries - Switzerland and Belgium. The area with concentrations 100 times less than that near the source spreads also over the Netherlands, Austria and covers the considerable part of Germany, and the Czech Republic.

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 residence time of PCP in the atmosphere, 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 source (as an example see Fig.3):

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

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

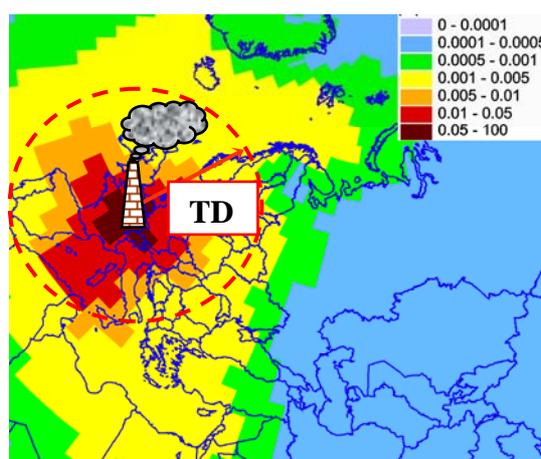It should be noted that such an approach is similar to that suggested in [*Rodan et al.*, 1999].

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. The calculated value of TD for PCP together with the half-life in the atmosphere is presented in Table 1.

Table 1. *Characteristics of LRTP (**Half-life in air_{calc}** and **Transport Distance**) calculated for PCP*

Substance	$T_{1/2}^{air}$, days	*TD*, km
PCP	7.4	2750

The presented quantitative LRTP characteristics of PCP meet the LRTP criteria of Executive Body Decision 1998/2.

2. PERSISTENCE IN THE ENVIRONMENT

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 the 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, *Klasmeier et al.,* 2006 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 PCP 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:

$$T_{1/2}{}^{env} = \ln2 \Big/ \sum k_i \cdot f_i \qquad\qquad (2)$$

Here fractions f_i 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 PCP between main environmental media and the values of their half-life in each particular medium due to degradation process.

The distribution of PCP 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 model assessment of annual media balance of PCP in comparison with its annual degradation balance is shown in Fig.4.

By the end of a year 1 tonne of PCP emitted to the atmosphere has degraded in all the media by about 75%. From this amount about 40% of emissions degraded in soil and about 25% – in the atmosphere. The bulk fraction of the pollutant remaining in the environment to the end of the year was accumulated in soil. Due to fast degradation of PCP in seawater the fraction of the pollutant accumulated in this media is negligible. Thus, model calculations allow us to demonstrate the re-distribution of PCP between main
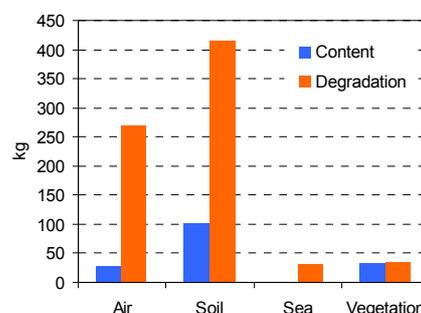

Fig. 4. *Annual degradation and media balances for PCP*

environmental media defining among them the media capable to accumulate the most part of the considered pollutant as well as those characterized by the most intensive degradation of the substance.

To evaluate the ability of the considered pollutant to be persistent in the environment, the values of **Half-life in the environment** were estimated on the basis of calculated media balance and the values of half-lives in the corresponding environmental compartments in accordance to formula (2). Obtained estimates of $T_{1/2}^{env}$ are presented in Table 2.

Table 2. *Characteristics of Persistence (Half-life in environment) and degradation half-lives of PCP in different environmental media*

Substance	$T_{1/2}^{env}$		Half-life, days		
	days	months	air	water	soil
PCP	45.7	≈ 1.5	26	2	48

The obtained value of $T_{1/2}^{env}$ shows that persistence of PCP in the environment can be characterised as relatively low.

3. COMPARISON WITH BENCHMARK SUBSTANCE

It should be noted that the obtained numerical values of $T_{1/2}^{air}$ and $T_{1/2}^{env}$ of particular chemicals are model dependent. One of the possible ways to exclude such dependence 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 its ranking in terms of persistence or LRTP among the well-known benchmark chemicals. Examples of chemical ranking and classification approach are described by *Matthies et al.* [1999], *Beyer et al.* [2000] and *Bennett et al.* [2001]. Benchmark approach may also be applicable for 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 PCP against those obtained for a benchmark pollutant is presented in this subsection. Benzo[a]pyrene (B[a]P) is used as a benchmark substance. Characteristics of its behaviour in the environment are well studied and clearly meet UN ECE criteria. It is already included in the CLRTAP Protocol on POPs and is considered as a pollutant of regional concern. Model calculations were performed for one-year period and a conventional point emission source with one and the same location in Europe and one and the same emissions intensity.

The comparison of the transport distances and half-lives in the environment for PCP and B[a]P is shown in Fig. 5 a and b.
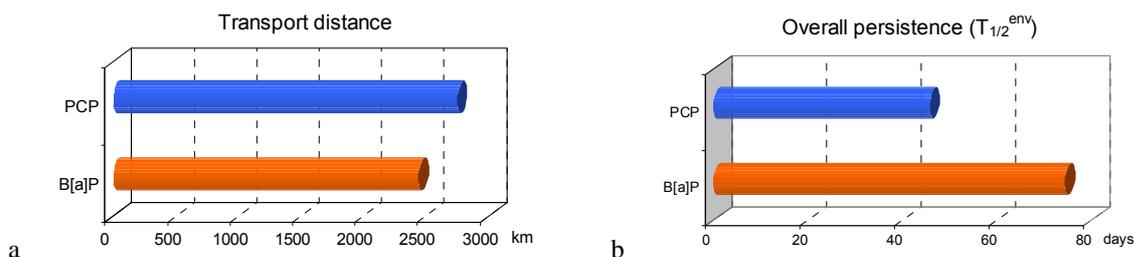
Fig. 5. *Transport distance and Half-life in the environment calculated for PCP and B[a]P*

According to the model calculations of *TD*, LRTP of PCP is slightly higher than that of B[a]P. The ranking of PCP and B[a]P with respect to $T_{1/2}^{env}$ shows that PCP is less persistent than B[a]P.

4. CONCLUDING REMARKS

The results of evaluation of LRTP and persistence for PCP by MSCE-POP model along with its physical-chemical properties are given in Table 3 in relation to the LRTP and persistence criteria outlined in the Executive Body Decision 1998/2.

Table 3. *Comparison of properties of PCP and criteria of **Executive Body Decision 1998/2** based on published data and with additions of MSCE-POP model outputs*

Criterion	Criterion values	Meets the criterion (Yes/No)	Characteristics of PCP	Remarks
Potential for Long-range Transboundary Atmospheric transport				
Vapour pressure, Pa	< 1000	Yes	0.0070 – 0.2131	*Borysiewicz*, 2008
			0.00415 – 0.50	*Mackay et al.*, 1997
			22.9	*Cahill et al.*, 2003
Half-life in air, days	> 2	Yes	26	Calculated on the basis of rate constant for vapor-phase reaction with hydroxyl radicals in air from *Howard and Meylan*, 1997
Half-life in air (calc), days		Yes	7.4	$T_{1/2}^{air}$ calculated by MSCE-POP
Persistence				
Half-life in water, months	> 2	No	0,76	*Cahill et al.*, 2003
			0.03 – 1.0	*Shamin et al.*, 2008
			0,01 – 7.8	*Mackay et al.*, 1997
Half-life in soil, months	> 6	No	0.2 – 2.1	*Shamin et al.*, 2008
			1.6	*Pesticide Properties in the Environment*, 1996
Half-life in the environment	-	-	1.5 months (45.7 days)	$T_{1/2}^{env}$ calculated by MSCE-POP
Bioaccumulation				
Log K_{ow}	> 5	Yes	5.12	*Mackay et al.*, 1997

The results of the model assessment demonstrate the considerable long-range atmospheric transport potential and relatively low persistence of PCP in the environment. This conclusion is also confirmed by the comparison of calculated numerical characteristics of LRTP and persistence of PCP against those obtained for typical POP of regional concern – B[a]P.

Thus, according to the results of the present investigation, PCP meets the LRTP criteria for POPs (calculated half-life in the atmosphere is 7.4 days). The persistence of PCP in the environment is about 1.5 months, which is slightly less tant 2 months but is of the same order of magnitude as of B[a]P.

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LEVELS OF PCP MEASURED IN ENVIRONMENTAL SAMPLES

Available data on the environmental concentrations of PCP are presented below.

Air concentrations

Literature data on PCP levels in the atmosphere are rather scarce. The results of investigation of atmospheric contamination in various Canadian regions in 1994 – 1996 are summarized in Table A1.

Table A1. *Levels of PCP in Canadian air*

Sampling location	Sampling data/period	Mean PCP, concentrations, ng/m^3	References	Remarks
Regina	May-July, 1994	0.30	*Cessna et al.*, 1997	South – central Saskatchewan
Agriculture and Agri-Food Canada Research Station (AAFC)	July-November 1995; January – May, 1996	0.4	*Waite et al.*, 1998	Located immediately south of the city of the Regina, representing a rural site on prairie farm land in south-central Saskatchewan
Waskesiu	May-July, 1994	0.23	*Cessna et al.,* 1997	Is a rural site in the Prince Albert National Park which in the boreal forest of central Saskatchewan
	July-November 1995; January – May, 1996	0.7	*Waite et al.*, 1998	
Prince Albert	July-November 1995; January – April, 1996	2.4	*Waite et al.*, 1998	Is a small city located 100 km south of Waskesiu at the edge of the boreal forest. It formerly had a wood treatment facility which used PCP and caused local soil contamination
Yellowknife	May-July, 1994	1.53	*Cessna et al.,* 1997	A small sity in the south-central Northwest Territiries, is the territirial goverment seat and has local mining activity
	July-November 1995; January – April, 1996	1.7	*Waite et al.,* 1998	
White City	July-November 1995; January – April, 1996	217.0	*Waite et al.*, 1998	A 'bedroom community' about 10 km east of Regina, is the location of an outdoor storage facility for PCP-treated utility poles transported from treatment facilities in Alberta or British Columbia.

The above data show rather low concentration levels in the majority of the considered regions. Considerably elevated levels were detected in the vicinity of the sources. For example, in White City maximum observed concentration is above 1 μg/m^3. Mean over sampling period at this location is also maximum among various locations.

The ability of long-range transport for pentachloroanisole (PCA), which is one of the main derivatives of PCP, is confirmed by measurement data at Arctic monitoring stations [*Su et al.,* 2008]. Pentachloroanisole – methyl pentachlorophenyl ether – was included into measurement program at 6 monitoring sites: Alert, Kinngait, Little Fox Lake in Canada, Point Barrow, USA, Zeppelin in Norway and Valkarkai in Russia. Air concentrations of pentachloroanisole showed strong seasonal/spatial variations with mean concentrations of 4.9 pg/m^3. Evidently, average levels of observed concentrations are low enough ranging from 0.5 to 10 pg/m^3.

Surface water

Investigations of contamination of surface waters and seas by pentachlorophenol were started in the middle of 70th last century. Particular interest was directed to the evaluation of PCP content in seawater. The results of inspection of the Baltic Sea in Gulf of Bothnia region in October 1982 and November 1983 are dicussed in [*Xie et al.,* 1986]. It was found that the obtained PCP concentrations ranged from 1 to 132 ng/L. Elevated concentrations were detected in upper layers at depth up to 2 m.

The data on marine environment monitoring by OSPARCOM in the North Sea region were summarized in the EuroClor report [*Pentachlorophenol. EuroChlor Risk Assessment for the Marine Environment*, 1999]

For coastal waters and estuaries of the North Sea, the concentrations were reported as either average (mean) or median PCP concentrations. On the whole, measured values were below 1 mkg/L, with a range of average/median concentrations from non detected to 0.79 mkg/L.

In estuary waters, average or median PCP concentrations have generally shown a decreasing trend with time during the period from 1983 to 1997. This decreasing trend reflect the better environmental management and the restrictions and bans imposed by various European countries on the use of PCP and its salts. Thus, considering all of the available monitoring data (covering the time period 1983 to 1997) the typical (or background) concentrations for coastal and marine waters are estimated to be 0.07 mkg/L [*Pentachlorophenol. EuroChlor Risk Assessment for the Marine Environment,* 1999].

The contamination of inland waters in Europe are characterized by wide concentration range from single units to several hundreds µg/l. High levels were observed in such industrial rivers as Rhine and Meuse. For their waters average or median PCP concentrations show generally decreasing trend during the period from 1976 to 1997. EuroChlor experts explain this by the prohibition of the usage of PCP and its derivatives as well as by other environmental-protection activities. Average or median PCP concentrations are generally lower on the eastern side of the North Sea (Netherlands and Germany) than on the western side (Great Britain).

In the beginning of 90th in Great Britain were detected three levels of PCP river contamination:

1. rivers in areas where PCP is not discharged, concentration range from 0.05 to 0.5 µg/L;

2. rivers in areas where PCP is used in industrial process and is regularly discharged, concentration range from 0.5 to 5 µg/L;

3. rivers as a result of a major pollution incident, concentration range from 5 to 50 µg/L.

Recent data (1995-1997) from numerous locations in Great Britain show concentrations at or below 0.1 mkg/L [*Pentachlorophenol. EuroChlor Risk Assessment for the Marine Environment*, 1999].

Soil

There are few investigations of soil contamination in regions located far from emission sources. The data on PCP content in rural soils and in soils in urban areas are absent.

In the humus layer of the Austrian Alps PCP concentrations range from < 1.0 to 2.1 mkg/kg. In soils in the Netherlands concentrations were detected at the same level < 1.0 mkg/kg. However, in soils in storage area of timber treatment plant the concentrations enlarge up to thousands mkg/kg [*Hazard Assessment*, 1995].

Investigations of PCP migration along soil profile in the area of timber treatment plant, where during the period of usage PCP for wood preservation very high levels of PCP contamination were formed, show that in such places most contamination relates not to surface soil but to soil at depth of 70 – 80 cm [*Troyanskaya et al., 1998*].

PHYSICAL-CHEMICAL PROPERTIES OF PCP USED FOR MODELLING

Some parameters needed for modelling of PCP atmospheric transport with their temperature dependencies were taken from the literature or from special databases. Physico-chemical properties for which literature data are absent were evaluated by known relations with other constancs, see Table B1.

Table B1. *PCP parameters used for atmospheric transport modelling*

Parameter (base values are given at 10º C)	Numerical value	Source
Henry's law constant for fresh water, Pa·m^3/mol	0.62	*Mackay et al.*, vol. V, 1997
Henry's law constant for seawater, Pa·m^3/mol	0.62	
Temperature coefficient for Henry's law constant, K	1300	NIST Chemistry Webbook, HSDB data base
Washout ratio	85 000	*van Pul et al.*, 1998
Vapor pressure over subcooled liquid, Pa	0.029	*Stepenson and Malanowski,* 1987
Temperature coefficient for vapor pressure, K	8303	
Second order degradation rate constant for reaction with OH-radical, cm^3/sec	4.61×10^{-13}	*Howard and Meylan*, 1997
Degradation in air constant, s^{-1}	3.06×10^{-7}	Estimated by the MSCE-POP model on the basis of [OH$^-$] distribution.
Half-life in air, days	26	
First order degradation rate constant for water, sec^{-1}	4.01×10^{-6}	Calculated using the data from ChemFate Search Results
Half-life in water, days	2	ChemFate Search Results
First order degradation rate constant for soil, sec^{-1}	1.67×10^{-7}	*Calculated using the data from HSDB and Pesticide Properties in the Environment*, 1996
Half-life in soil, days	48	*HSDB database, Pesticide Properties in the Environment*, 1996
Molar volume, cm^3/mol	162.4	*Jaw et al.*, 1999
Octanol/water partitioning coefficient, K_{ow}	1.318×10^5	*Howard and Meylan*, 1997
Octanol/air partitioning coefficient, K_{oa}	4.2×10^8	Estimated on the basis of relation between K_{oa}, K_{ow} and K_{aw}
Temperature coefficient for K_{oa}, K	1300	
Molecular diffusion coefficients, m^2/sec:		
for water	7.52×10^{-10}	Calculated with the help of equations from *Schwarzenbach et al.*, 1993
for air	6.27×10^{-6}	
Partitioning coefficient in the system organic carbon/water, m^3/kg	5.37×10^3	Calculated with the help of relationship between K_{OC} and K_{OW} given in *Karikhoff,* 1981