

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 Dicofol

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INTRODUCTION

Dicofol is an organochlorine pesticide of widespread occurrence. Chemicals with different trade names (Kelthane, Hifol, Milbol et al.) and different content of dicofol were used in agriculture. In addition mixtures of dicofol with other pesticides were used. Dicofol is a miticide and broad-spectrum non-systematic acaricide with little insecticidal activity. It is used on terrestrial food crops and non-food sites [RED Dicofol, 1998].

Dicofol is included into the OSPAR List of Chemicals for Priority Action (Update 2004) [Meeting of the OSPAR Commission (OSPAR), 2004]. As a potential candidate for the inclusion into the UN-ECE Protocol on POPs this chemical was addressed by the Ad Hoc Expert Group on POPs [Lerche et al., 2002]. This year the Netherlands has re-submitted the dossier on dicofol [van de Plassche and Rasenberg, 2003] for technical review by the Task Force on POPs. Additional information for the evaluation of dicofol as a potential new POP 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 pollutants, EMEP/MSCE-POP multicompartiment hemispheric transport model is used. To estimate the considered parameters for dicofol, the model calculation of its atmospheric transport from a conventional emission source located in Europe is made for one-year period. Since dicofol is a pesticide its emissions to the atmosphere occur as a result of its application on crop areas. In this connection, a conventional diffusive emission source covered the use area of approximately 200 by 200 km is considered. Information on physical-chemical properties and degradation rates of dicofol used for modelling is included in Annex. Of note, in this model assessment dicofol was treated not as one compound - p,p'-isomer but as the technical product - a mixture of two isomers (p,p'- and o,p'-dicofol).

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

Persistence in the environment is evaluated by **Half-life in the environment** ($T_{1/2}^{env}$) estimated for dicofol 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 dicofol with the help of the model dependent TD and $T_{1/2}^{env}$, a comparison of their numerical values against those obtained for adequately studied "benchmark substance" B[a]P is presented.

In conclusion, the calculated numerical characteristics of LRTP and persistence of dicofol 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_{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. 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 dicofol 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 atmospheric transport of dicofol 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 dicofol to the atmosphere are assumed to be 1 tonne per year from a conventional diffusive emission source with the use area of approximately 200 by 200 km and located in Europe (with centre in 10°E; 47.5°N). On the basis of this calculation annual atmospheric balance of the removal of dicofol from the atmosphere is estimated. The calculated balance of dicofol removal from the atmosphere is given in Fig.1.

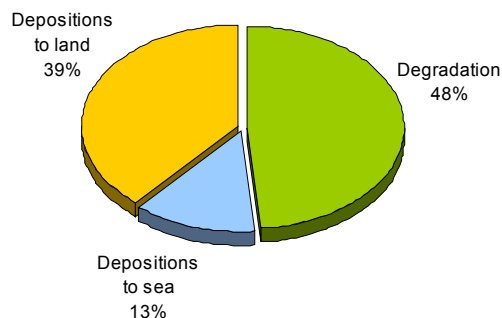


Figure 1. Calculated annual balance of dicofol removal from the atmosphere

According to the model assessment, processes of degradation and depositions to different types of underlying surfaces contribute almost equally to the removal of dicofol from the atmosphere and produce equal effect on the calculated value of $T_{1/2}^{air}$. 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. As seen from the balance, dicofol removal from the atmosphere due to deposition processes to soil is three times more intensive and affects LRTP of this pollutant to a greater extent than deposition to the sea surface.

In this model assessment degradation process of dicofol in the atmosphere is considered as the gas-phase interaction with photochemically – produced hydroxyl radicals and all other reactions are neglected. In the literature the half-life for this reaction is estimated to be 3.1 [Syracuse database, 2000 cited by *van de Plassche and Rasenberg, 2003*] and 4.7 days [HSDB, 2001]. For the model calculation of $T_{1/2}^{air}$, literary data on second-order degradation rate constant for the gas-phase of dicofol equal to $3.43 \cdot 10^{-12} \text{ cm}^3/\text{molec}\cdot\text{s}$ and derived using a structure estimation method [Howard and Meylan, 1997; HSDB, 2001] are used. The residence time of dicofol in the atmosphere ($T_{1/2}^{air}$) estimated on the basis of model calculations of its atmospheric transport totals to three days. The numerical value of this characteristic of LRTP for this compound fully 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 dicofol is provided by the spatial distribution of its air pollution obtained also on the basis of simulation of its atmospheric transport from conventional diffusive emission source and calculated atmospheric balance. In Fig 2 concentration fields of dicofol 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.

With a conventional diffusive source of emissions located in Europe, the area of atmospheric air concentration of dicofol, which is 1000 times lower than the concentration near the source, is located over the most part of the Central Europe and the UK, includes Mediterranean Sea and Eastern Europe and reaches southern part of the Scandinavian Peninsula, northern Africa and middle-Atlantic. Considering the influence of the emission source on the EMEP domain in more detail (see Fig.2b)

shows that the most intensive air pollution by dicofol 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, Italy and the Czech Republic.

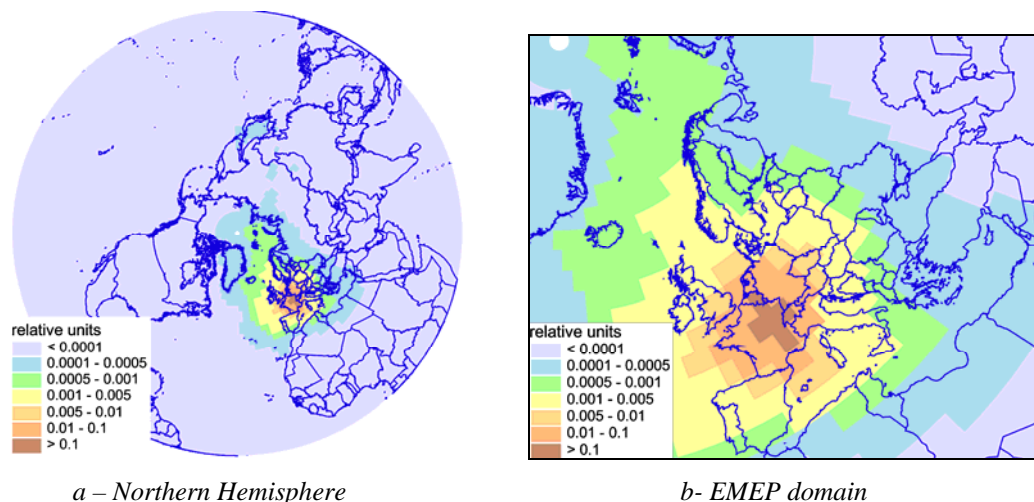


Fig. 2. Spatial distribution of dicofol concentrations in the above-ground air in the Northern Hemisphere and in the EMEP domain

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 dicofol 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):

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

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].

Transport distance is the second numerical characteristic of LRTP obtained by the model calculations. The value of *TD* obtained by calculations depends on the processes removing the pollutant from the

atmosphere. These are deposition to the underlying surface (land, sea) and atmospheric degradation. The calculated value of *TD* for dicofol occurs to be **1650 km**.

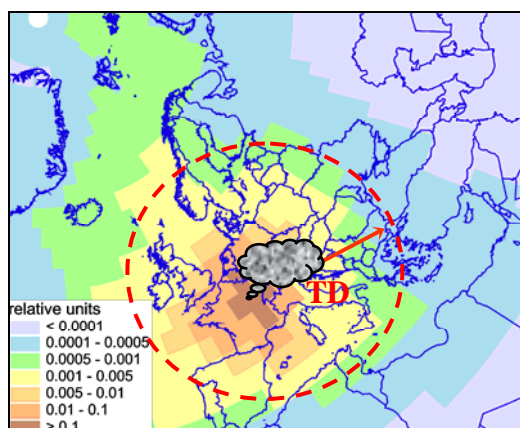


Fig.3. Definition of the transport distance

Both characteristics of LRTP obtained for dicofol with the help of model calculations are presented in Table 1.

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

Substance	$T_{1/2}^{air}$, days	<i>TD</i> , km
Dicofol	3	1650

The presented quantitative characteristics of dicofol LRTP 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, 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 dicofol 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 dicofol between main environmental media (air, soil, water, sediment and vegetation) and the values of their half-life in each particular medium due to degradation process.

Hydrolysis is expected to be an important fate process for dicofol with half-life value, which at pH 7 amounts less than 3 days. With decrease of pH up to 5 the value of hydrolysis half-life for the considered pollutant rises steeply up to 85 days [HSDB, 2001]. According to the data of Spray Material Half-life Chart 2005 the half-life of dicofol at pH 7 totals to 5 days; at pH 5 – 20 days. Thus, dicofol may be substantially more persistent in some acidic water, particularly in those with relative long hydrological residence times and low microbiological populations [RED Dicofol, 1998]. Data on acidity of surface water in the European and US countries available at present testify that water bodies are not acidic with pH values typically around 7- 8. However, there are sensitive, ecologically valuable water bodies in some regions in many countries with lower, more acidic pH values [van de Plassche and Rasenberg, 2003]. That is why, for the sake of model parameterisation half-life of dicofol in water was taken as an average value between available data for the interval of pH from 5 to 7, i.e. 30 days. Besides, the half-life of dicofol in water depends not only upon the above-mentioned hydrolysis but also on the life activity of organisms and intensity of ultraviolet radiation. For soluble dicofol, photolysis may be important degradation pathway. The half-life for this reaction is 37 days.

The different estimates of dicofol persistence in soil can be found in various literary sources. The scattering of data on half-life of dicofol in soil available in the literature is reflected in Table 2.

Table 2. Dicofol half-life in soil and bottom sediment

Half-life, days	Notes	References
45		<i>Pesticide Properties in the Environment</i> , [1996]
66.4	Aerobic soil	<i>PAN Pesticides Database - Chemicals</i>
203		<i>ARS pesticide properties</i> , at pH=7.8
15.9	Anaerobic soil	<i>PAN Pesticides Database - Chemicals</i>
16		<i>ARS pesticide properties</i> , at pH=7.8
60		
15.9	Anaerobic soil condition	EXTOXNET
30	Silty loam, photodegradation	
58	California cotton fields, irrigated soil	HSDB, 2001
113	Florida, citrus groves	
90	New York, apple orchards	
43	Silty loam, biodegradation	
194 – 345	Bottom sediment and soil at aerobic conditions	
30	Bottom sediment and soil at anaerobic conditions	

Laboratory and field studies indicate that dicofol has a short to intermediate half-life and is moderately persistent in the environment as a result of normal label use [HSDB, 2001]. Since substances classified as moderately persistent have half-life values amounting from 30 to 100 days, half-life of dicofol in soil equal to 60 days was taken for model parameterisation. Besides, of note, the technical product for the most part contains p,p'-dicofol (80%), which is more persistent in soil than o,p'-isomer.

For dicofol the distribution of its 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 dicofol in comparison with its annual degradation balance is shown in Fig.4.

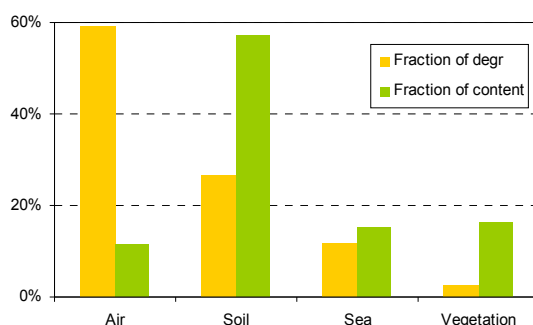


Fig. 4. Annual degradation and media balances for dicofol

By the end of a year 1 tonne of dicofol emitted to the atmosphere has degraded in this medium more than by half. At that the degradation of dicofol amount appeared to be in soil due to intermedia exchange processes between the atmosphere and soil is equal to almost 30%. The contribution of vegetation to dicofol degradation is practically negligible amounting to 2%, the relative fraction of the pollutant degraded in sea is somewhat higher totalling to 12%. At that more than a half of overall dicofol content in the environment is accumulated in soil, 10% remain in the air, the rest part of the pollutant is distributed in the following way: seawater – 15%, and vegetation – 16%. Thus, model calculations allow us to demonstrate the re-distribution of dicofol between main 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.

Calculated value of *Half-life in the environment* for dicofol is equal to 20 days (or 0.7 month). The obtained estimate of $T_{1/2}^{env}$ together with values of half-life in the separate environmental media used for modelling (for references please see Annex A) are presented in Table 3.

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

Substance	$T_{1/2}^{env}$		Half-life, days		
	days	months	air	water	soil
Dicofol	20	0.7	3	30	60

The obtained value of $T_{1/2}^{env}$ shows that persistence of dicofol in the environment is relatively not high. Also it should be noted that value of $T_{1/2}^{env}$ is lower than those of half-life in water and soil, which take into account degradation processes only.

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 Pov 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]. 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 dicofol 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. 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 diffusive source with one and the same location in Europe and one and the same emissions intensity.

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

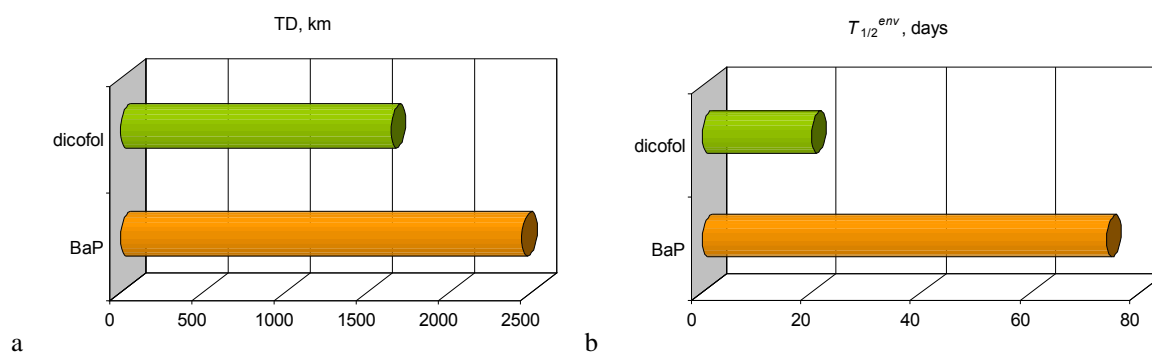


Fig. 5. Half-life in the environment and Transport distance calculated for dicofol and B[a]P

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

Thus, according to the results of the present investigation, dicofol meets the LRTP criteria for POPs.

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

In Table 4 dicofol properties presented in [van de Plassche and Rasenberg, 2003] are compared to criteria of Executive Body Decision 1998/2 with additions of the MSCE-POP model outputs. Data on physical-chemical properties of dicofol available in [van de Plassche and Rasenberg, 2003] and used in the model calculations are given in the Annex (Tables A1 and A2).

Table 4. Comparison of properties of dicofol and criteria of Executive Body Decision 1998/2 based on data [van de Plassche and Rasenberg, 2003] and with additions of MSCE-POP model outputs

Criterion	Criterion values	Meets the criterion (Yes/No)	Characteristics of dicofol	Remarks
Potential for Long-range Transboundary Atmospheric transport				
Vapour pressure, Pa	<1000	Yes	5.3×10^{-5}	Presented in van de Plassche and Rasenberg, 2003
Half-life in air, days	>2	Yes	3.1 – gas phase; 3.5 – 10 - particles	
Half-life in aircalc, days		Yes	3	$T_{1/2}^{air}$ calculated by MSC-E
Persistence				
Half-life in water, months	>2	Yes	Half-life o,p'-isomer: 47; 0.3 and <0.1 days for pH 5, 7, and 9. Half-life p,p'-isomer: 85, 4 and <0.1 days for pH 5, 7 and 9.	Presented in van de Plassche and Rasenberg, 2003
Half-life in soil, months	>6	No	Half-life o,p'-isomer: 8-35 days. Half-life p,p'-isomer; 21-60 days.	
Half-life in sediments, months	>6	No	Half-life < 1 day for p,p'-isomer and p,p'-isomer (pH water phase 7.6-7.8).	
Half-life in the environment, months	-	-	0.7 months (20 days)	$T_{1/2}^{env}$ calculated by MSC-E

The results of the model assessment demonstrate the considerable long-range atmospheric transport potential and relatively low persistence of dicofol 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, it should be noted that in this model assessment the behaviour of dicofol in the environment was studied as for the mixture of two isomers. Besides, due to the lack of available data on dicofol isomers in the literature, the model estimates are obtained not taking into account temperature dependence of their key physical-chemical properties such as subcooled liquid-vapour pressure, the Henry's law constant, and partition coefficients. In this connection the obtained model results should be considered as preliminary.

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PHYSICAL-CHEMICAL PROPERTIES OF DICOFOL USED FOR MODELLING

In industry dicofol manufacture begins with DDT dehydrochlorination and the received product is sequentially chlorinated and treated with hydrochloric acid. As a result a mixture of p,p'-dicofol (~80%) and o,p'-dicofol (~20%) is produced. In addition the technical product always has admixtures such as metabolites of DDT and its derivatives as well as other compounds. 18 species in all have been identified [Clark, 1990]. Modern manufacturing processes can produce technical grade dicofol which contains less than 0.1% DDT [EXTOXNET]. In this model assessment dicofol was treated not as one compound - p,p'-isomer but as the technical product - a mixture of two isomers. Obviously presence of admixtures in the preparation, first of all of o,p'-isomer, should influence its physical-chemical properties. At present in the literature, values of saturated vapour pressure, solubility etc. are given for the technical product. Therefore, for further understanding of the behaviour of the substance in the environment more detail investigation of key physical-chemical properties of the dicofol isomers is needed.

Key physical-chemical properties of dicofol presented in [van de Plassche and Rasenberg, 2003] are shown in Table A1.

Table A1. Physical-chemical properties of dicofol presented in [van de Plassche and Rasenberg, 2003]

Physical chemical properties	Numerical values
Vapour pressure, Pa	$5.3 \cdot 10^{-5}$ [1]
Henry's law constant, Pa·m ³ /mol	-
Octanol-water partition coefficient (log K_{OW})	4.08 – 5.02 – various sources
Half-life, days	
Air	3.1 [2]
Water	Hydrolysis half-life o,p'-isomer: 47; 0.3 and <0.1 days for pH 5; 7; and 9. Hydrolysis half-life p,p'-isomer: 85; 4 and <0.1 days for pH 5; 7 and 9. Photodegradation half-life o,p'-isomer – 1.5 and 14.8 days for sensitised and non-sensitised conditions. Photodegradation half-life p,p'-isomer - 4 and 92.5 days, respectively [3].
Soil	On silt loam soil irradiated with artificial light half-life o,p'-isomer- 30 days, half-life p,p'-isomer-21-30 days [4]. In a silt loam half-life p,p'-isomer of 43 days, in anaerobic conditions – 30 days [5]. O,p'-dicofol degraded in aerobic soil with a half-life of 8 days in a loam soil. Under anaerobic condition o,p'-dicofol degraded with a half-life of 6 days from a flooded silt loam soil [4]. Field dissipation studies total parent – $t_{1/2}$ = 62 days at pH 8.4-8.9 (Kelthan 35); $t_{1/2}$ = 3.7 days at pH 6.3-7.2 (Kelthan MF). p,p'-dicofol - $t_{1/2}$ = 50-60 days and o,p'-dicofol - $t_{1/2}$ = 30-35 days at pH 7 (Kelthan APS NEW) [3].
Sediment	Half-life o,p'-isomer: 0.31-54 days. Half-life p,p'-isomer: 0.05-0.06 days

Note: 1 - Pesticide Manual; 2 - Syracuse Database; 3 - IUCLID dataset; 4 - EPA RED; 5 - MRID 41050701

Since the temperature dependences of all physical-chemical properties and degradation rates of dicofol were not found in the literature, the analysis of available data did not allow us to prepare the “traditional” model parameterisation as it is made in MSCE-POP model usually. The set of dicofol properties used for the model assessment is presented in Table A2.

Table A2. Physical-chemical properties of dicofol used for modelling of its atmospheric transport

Physical-chemical properties	Values at 25 °C	References
Henry' s law constant for fresh water, Pa m ³ /mol	0.0244	HSDB, 2001
Henry' s law constant for marine water, Pa m ³ /mol	0.0244	
Coefficient of Henry's law constant temperature dependences, K	-	
Washout ratio	20 000	Selected value correspond Washout ratio for p,p'-DDT
Subcooled liquid-vapour pressure, Pa	$3.07 \cdot 10^{-4}$	Estimated on Ps at 25 °C Mackay et al. [1997], vol.V
Coefficient of subcooled liquid-vapour pressure temperature dependences, K	-	
Rate constant of the reaction with OH-radical in air, cm ³ /c	$3.43 \cdot 10^{-12}$	Howard and Meylan, 1997
Half-life in air, days	3	Calc with the use of average value of OH- spatial distribution used in the model: [OH] = 8.8×10^5 molecule/cm ³
Degradation rate constant in water, c ⁻¹	$2.14 \cdot 10^{-7}$	Selected value on data from HSDB, 2001
Half-life in water, months	1	
Degradation rate constant in soil, c ⁻¹	$1.34 \cdot 10^{-7}$	
Half-life in soil, months	2	
Molar volume, cm ³ /моль	333.5	Molar volume for p,p'-DDT, Mackay et al. [1997], vol.V
«Octanol-water» partition coefficient	19100	HSDB, 2001
«Octanol-air» partition coefficient	$1.95 \cdot 10^9$	Estimated
Coefficient of «octanol-air» partition coefficient temperature dependence, K	-	
Molecular diffusion coefficients, m ² /s:		Calculated with the help of equations from Schwarzenbach et al., 1993
in water	$4.92 \cdot 10^{-10}$	
in air	$4.49 \cdot 10^{-6}$	
“Organic carbon-water” partition coefficient, m ³ /kg	7.812	Calculated with the help of relationship between K _{OC} and K _{OW} given in Karickhoff [1981]