ESTIMATED TRANSFER OF VOLATILE ORGANOCHLORINE SUBSTANCES IN THE ECOSYSTEMS WATER, SEDIMENT, BIOTA USING THE CONCEPT OF FUGACITY

Mihaela Iordache[1], Luisa Roxana Popescu[1,2], Luoana Florentina Pascu[3], Ioan Iordache[4*]

[1]*National Research and Development Institute for Industrial Ecology – INCD-ECOIND Bucharest-Subsidiary Ramnicu Valcea, 1 Uzinei Street, Ramnicu Valcea 240050, Romania;* [2]*University "Politehnica" of Bucharest, Faculty of Applied Chemistry and Material Science, Gh. Polizu 1-7, 011061, Bucharest, Romania;* [3]*National Research and Development Institute for Industrial Ecology – Bucharest, 71-73 Podu Dambovitei Street, 060650, Bucharest, Romania;* [4]*National Research and Development Institute for Cryogenics and Isotopic Technologies - ICSI Rm. Valcea, Uzinei Street no. 4, P.O. Box Râureni 7, 240050, Râmnicu Vâlcea*

ABSTRACT

This aims of this paper is to studying the transfer of organochlorine substances (1, 2-dichloroethane, trichlorethylene, perchlorethylene and 1,2,4-trichlorobenzene) in the environmental water, sediment and biota using calculation MacKay model. The water/sediment samples were collected from the Olt River, in two locations, Cremenari and Babeni Marcea, situated downstream of the industrial platform Ramnicu Valcea, during 2013-2014. Modelling revealed clear trend the transfer of component "air" of these pollutants are known fact that volatile compounds, however, based on modelling was observed a significant transfer of these pollutants in the factor "biota" in amounts which may generate medium and long term risk to human health by taking in the food chain, which at first sight and a first risk assessment made by these pollutants for local residents can go unnoticed.

Keywords: volatile organochlorine substances, MacKay model, fugacity, ecosystem

1. INTRODUCTION

Pollution represents a threat to the economic development and human health and environmental protection [IP/A/ENVI/ST, 2007]. Hazardous substances pollution is due to wastewater discharges from point sources and diffuse emission sources that contain non-synthetic pollutants (heavy metals) and/or synthetic pollutants (organic micro-pollutants). Hazardous substances produce toxicity, persistence and bioaccumulation in the aquatic environment. Volatile organic compound are widely used in industry, given their ability evaporation after use. The large amounts of organochlorine substances are obtained during the

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chlorination of drinking water and wastewater. Although it was found that over 200 natural halogenated hydrocarbons are obtained, most chlorinated compounds that are released into the environment or fabricating in the environment, are of anthropogenic origin. These products manufactured by man have led to the contamination of air, soil and water. 1,2-dichloroethane is one of the most widespread of xenobiotic compounds present in industrial wastewater discharges in the ground water and soil [Fewson C. A. et al., 1981]. The use of volatile organic compounds is not without risks for the environment and therefore, precautions must be taken to treat the air it contains. The accession of Romania to the European Union in 2007, and thereby align with the European legislation, determine Romania to adopt major changes to how the issues related to environmental pollution. The Water Framework Directive (2000/60/EC) introduced in 2000, and ambitious new targets for protecting and restoring aquatic ecosystems as a basis for ensuring sustainable water use in the long term for people, the economy and nature. In order to establish effective control of water pollution, the Directive provides a common objective for all countries implementing it: achieve "good ecological and chemical quality" water by 2015. Water Framework Directive (2000/60/EC) includes objectives for good ecological and chemical status of surface waters and good chemical and quantitative status of groundwater and was transposed into national law by Law no. 310/2004 for amending Law No. 107/1996. In The decision No. 1038/2010 on "the approval of the measures against pollution with chemicals", the organochlorine substances: 1, 2-dichloroethane, trichlorethylene, 1, 2, 4 trichlorobenzene and perchlorethylene belong to the "List I" of priority substances. Justification for selection and classification of these substances in the environment resides in their behavior. They do not degrade, but persist in the environment and accumulate in animal and plant tissues, thus showing, long-term risks to human health and ecosystems. As these substances progresses in the food chain, their concentration increases risks to human and ecosystem following the same trajectory. It is therefore necessary to take control of emissions of these substances, even when they are very small [Proiect PC, 2001-2006; Dyck R. et al. 2011; Vasquez V.R. et al. 2011& Alamdar A. et al. 2014]. One way to estimate the level of pollution with hazardous chemicals to environmental water, sediment, biota is Model MacKay. This model can give hints conclusive for a rapid risk assessment on which to base conclusions on the preventive measures for the future studied area. Effective management requires understanding of the environment and the ability to analyse quantitative risk transfer mechanism associated health and chemical contamination. The level of contamination resulting from accidental chemical discharges or continuous was usually assessed using transfer models on environmental compartments. These models are mainly based on a single environmental compartment, such as the transfer of a contaminant in water. However, the chemicals that are released into the environment, succeed through various compartments of the environment as a result of complex processes physico - chemical and biological [Warren C. et al., 2005; Luo Y. et al., 2007; Gokgoz-Kilic S., Aral M. M., 2008; Dong J. et al., 2009; Zhang Y. – Z. et al., 2011; Luo X. et al., 2015]. One such model is the MacKay model [Mackay D., Paterson S., 1981 & Mackay D., 1991], which uses patterned backgrounds to explore the possible

behaviour of the chemical. For this purpose model generates some equations that can be validated using real environments. A somewhat different assembly equation proves to be convenient for real-world environments, but the basic principles are the same. Mackay model Level I is based on four basic components: air, water, sediment, soil and to, through bio-concentration factors can be added and biota. This calculation model is based on using its fugacity and can quickly estimate the level of pollution in the environment with pollutants analysed without carrying out analytical determinations costly in terms of time and money.

The purpose of the present study was to studying the transfer of organochloride substances (1, 2-dichloroethane, trichloroethylene, perchlorethylene and 1, 2, 4-trichlorobenzene) in the environmental water, sediment and biota using calculation MacKay model.

2. MATERIALS AND METHODS

2.1. General data regarding the fugacity concept

In order to study distribution of chemicals in various environmental matrices was required and a qualitative description of the types of matrices, highlighting some of the most important properties of them. In this sense, they put together averages "model" that could be used later in the calculations. This was considered such an area of 1km / 1km including air, water, soils and sediments. These environments have been assigned volumes and typical properties, purely illustrative and that, in turn necessitated some changes if was treated chemical evolution in a specific region [Mackay D., 1991 & Zhang Y. - Z. et al., 2011]. These environments are shown in figure 1 for a better understanding of these environments or "unity of the world."
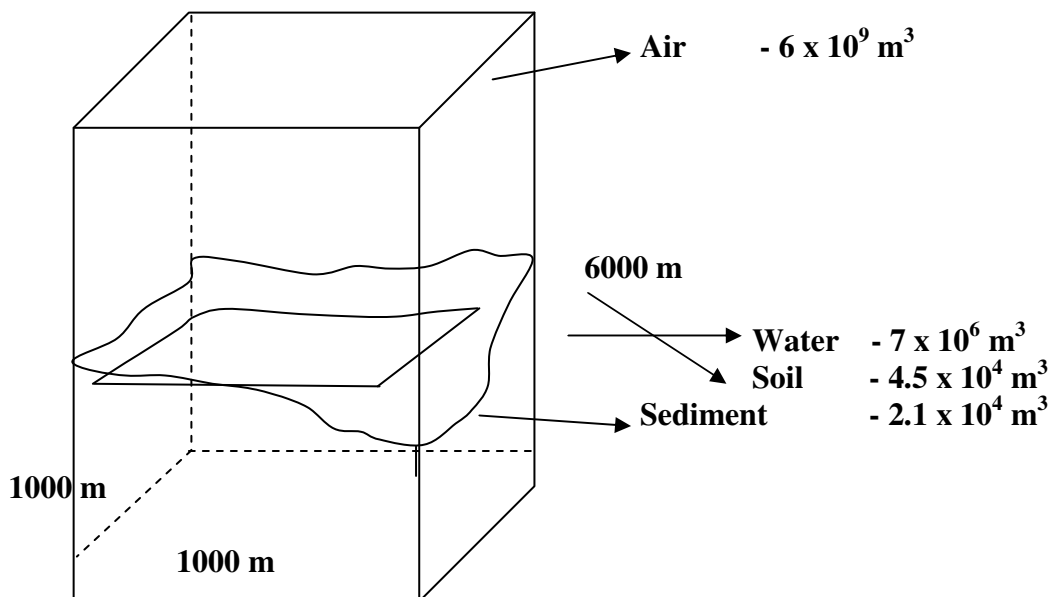

Air   - 6×10^9 m^3

6000 m

Water   - 7×10^6 m^3
Soil   - 4.5×10^4 m^3
Sediment - 2.1×10^4 m^3

1000 m

1000 m

Figure 1. "The unity of world" MacKay fugacity model - simple model with four compartments [Mackay D., 1991]

According to G.N. Lewis, fugacity concept describes the tendency of a chemical transition from one phase to another when they are in contact. It is identical to the concept of ideal gas partial pressure and chemical potential is related to logarithmically, so it varies linearly or non-linearly with concentration. At low partial pressures ideal conditions fugacity is equal to the partial pressure.

Based on the concept of fugacity, one can postulate a nearly linear relationship between fugacity dependence and concentration of the chemical in each environmental compartment (eq.1) [D. Mackay et al., 1981]:

$$C = Zf \tag{1}$$

where Z is a constant of proportionality called "fugacity capacity" with the units mol / m^3Pa. This equation implies that C always varies linearly with f. Nonlinearity can be adapted by consideration of Z as a function of C or f.

Fugacity (Z) for air [D. Mackay et al., 1981]

The basic equation for the fugacity for a substance in the state of the vapor (eq.2):

$$F = y \times \phi \times P_T \tag{2}$$

where y is the mole fraction of chemicals and fugacity coefficient Φ is P_T is the pressure (atmospheric) total.

If the law of gases (eq.3):

$$P_T V = nRT \tag{3}$$

where n is the total number of moles of air and chemicals present, and T is the absolute temperature, chemical concentration C (solute) will be that (eq.4-6):

$$C = \frac{yP_T}{RT} = \left(\frac{1}{\phi RT}\right)f \tag{4}$$

Thus Z is $\dfrac{1}{\phi RT}$ \hfill (5)

or

$$\frac{1}{RT} \tag{6}$$

when the $\phi = 1$.

Fugacity (Z) for water [Mackay D., Paterson S., 1981]

Fugacity equation for a compound «i» dissolved in water or another solvent is given in terms of mole fraction "xi", activity coefficient "γi" and reference

fugacity "fR" based on Raoult law as (eq. 7-14):

$$f_i = x_i y_i fR \tag{7}$$

$$C_i = \frac{n_i}{(V_w + V_i)} \approx \frac{n_i}{V_w} \tag{8}$$

$$V_w = n_w v_w \tag{9}$$

$$x_i = \frac{n_i}{n_i + n_w} \approx \frac{n_i}{n_w} \tag{10}$$

«i» - solute, and «w» - water

$$C_i \approx \frac{x_i}{v_w} \approx \frac{x_i}{(18 \times 10^{-6} m^3 / mol)} \tag{11}$$

$$f_i = C_i v_m y_i fR \tag{12}$$

or

$$C_i = \frac{1}{(v_w y_i fR) f_i} \tag{13}$$

$$Z_i = \frac{1}{v_w y_i fR} \tag{14}$$

For a solution in water ZW may be inferred as (eq. 15-17):

$$Z_w = \frac{1}{v_W y_i P_{SL}} \tag{15}$$

$$K_{AW} = \frac{Z_A}{Z_W} = \frac{H}{RT} = \frac{P_S}{C_S RT} \tag{16}$$

$$Z_w = \frac{Z_A RT}{H} = \frac{1}{H} = \frac{C_S}{P_S} \tag{17} \quad \text{(because } Z_A = \frac{1}{RT} \text{),}$$

C_S and P_S situation where are values for liquids and solids status.

Fugacity (Z) for the soil or sediment [Mackay D., Paterson S., 1981]

The simplest method of deduction of Z is correlating him for Z_{APA} using a dimensionless partition coefficient. This coefficient can be determined from several isothermal equations (linear, Langmuir, Freundlich). In most cases the data may be

represented, at least at low concentrations of the linear expression (eq. 18):

$$C_s = K_{SW} C_W \tag{18}$$

where C_S is the concentration of adsorbed (mol/m^3 of sorbent), C_W is the water content. The nonlinear equation KSW is a function of concentration. K_{SW} is a dimensionless partition coefficient.

As is known concentrations to adsorbed substances are usually expressed as the amount of solute (sorbent) adsorbed per unit mass. K_P is defined by units of L/kg and K_{SW} is related to the density of sorbent ρS in l g/L (or g/cm^3 or mg/m^3) as follows (eq. 19-22):

$$K_{SW} = \rho_S K_p \tag{19}$$

$$K_{SW} = \frac{Z_S}{Z_W} \tag{20}$$

$$Z_S = Z_W K_{SW} = \frac{\rho_S K_P}{H} \tag{21}$$

Fugacity (Z) for biotic phase (fish) [Mackay D., Paterson S., 1981]

$$Z_B = \frac{\rho_B K_{BW}}{H} \tag{22}$$

ρB equals the numerical density of water and can be ignored. It should be recalled, however, in cases where K_{BW} is defined on a dry weight basis (not wet mass), or the concentration in specific tissues such as fat. In these cases the density is calculated as the mass of biota / dry tissue per unit volume of wet biota.

If you develop procedures for estimating the Z values for each environmental situation again, then the equilibrium concentrations can be derived using f as a common criterion of balance.

Table 1. Defining the fugacity capacities [Mackay D., Paterson S., 1981]

Compartment	Definition Z (mol/m^3 Pa)
Air	1/RT ; R=8,314 Pa m^3/mol K ; T=Temp (K)
Water	1/H sau C^S/P^S C^S = aqueous solubility (mol/m^3) P^S = vapor pressure (Pa) H = Henry law constant (Pa m^3/mol)
Solid sorbent (e.g. : soil, sediment, particulate)	K_P ρ_S /H K_P= partition coefficient (L/kg) ρ_S = density (kg/L)
Biota	K_B ρ_B /H K_B= bioconcentration factor (L/kg) ρ_B = density (kg/L)
Pure solute	1/P^S v ; v= the molar volume of solute (m^3/mol)

2.2. Studied area

This area is located at south at 12 km of the city of Ramnicu Valcea and in a closer vicinity of an industrial platform (fig. 2). Two companies producing chemicals, a power plant and other industrial societies carries out its activity in the industrial platform. The water/sediment samples were collected from the Olt River, in two locations during 2013-2014. Sections examined in this study are located downstream of the industrial platform Ramnicu Valcea: Cremenari 44°58'50"N, 24°16'56"E; and Babeni-Marcea (M), 44°55'3"N, 24°14'52"E. Cremenari section is situated at approx. 8-10 km from industrial platform, while section Babeni-Marcea is located approx. 12 km from Cremenari section. The Olt River is one of the most important rivers in Romania and is the largest and the longest Romanian tributary of the Danube River.

2.3. Determination of organochlorine compounds

2.3.1. Determination of organochlorine compounds in water samples

The contents of organochloride compounds were determined by gas chromatography coupled with mass spectrometry (GS-MS).

A sample was taken and discarded glass bottle filled with enough water so that there was no residual sample volume of 200 mL. Add to the sample the extraction solvent (pentane), close and vigorously mix using a magnetic shaker or a mechanical shaker for 5 minutes to ensure that the extracting has been finely dispersed in the sample in order to obtain a reproducible recovery.

Determination of 1, 2, 4 -trichlorobenzene
Samples of water were taken in a brown glass bottle. The pH was verified and, if necessary, adjusted immediately after collection, to be within the range of 5 to 7.5. In order to prevent decomposition of the sample, the samples were carefully taken as soon as possible (preferably within 24 hours).

The sample volume was one litter. A volume of 30 mL of extraction solvent (heptane) was added and the solution was stirred for at least 10 minutes and transferred to a separating funnel with adequate capacity and standing to allow phase separation.

2.3.2. Organochlorine compounds determination in sediment samples

For samples that contain volatile components no any pre-treatment was necessary. Amount of 30 grams of wet soil was weighted in a glass iodometrical beaker. 50 mL of methanol were added and stirred 30 min., and then a volume of 50 mL pentane was added and stirred for another 30 min. The liquid phase was filtered through a filter paper with medium porosity and was introduced into a 500 mL separator funnel together with 250 mL distilled water. The soil was washed with 10 mL pentane. The funnel was stirred 5 min. allowing separation and discard

the organic phase. The organic layer was passed through a filter with anhydrous Na$_2$SO$_4$ into a hermetic closed vessel. The funnel and the layer with Na$_2$SO$_4$ was rinsed with 5 mL of pentane and added to the organic layer.
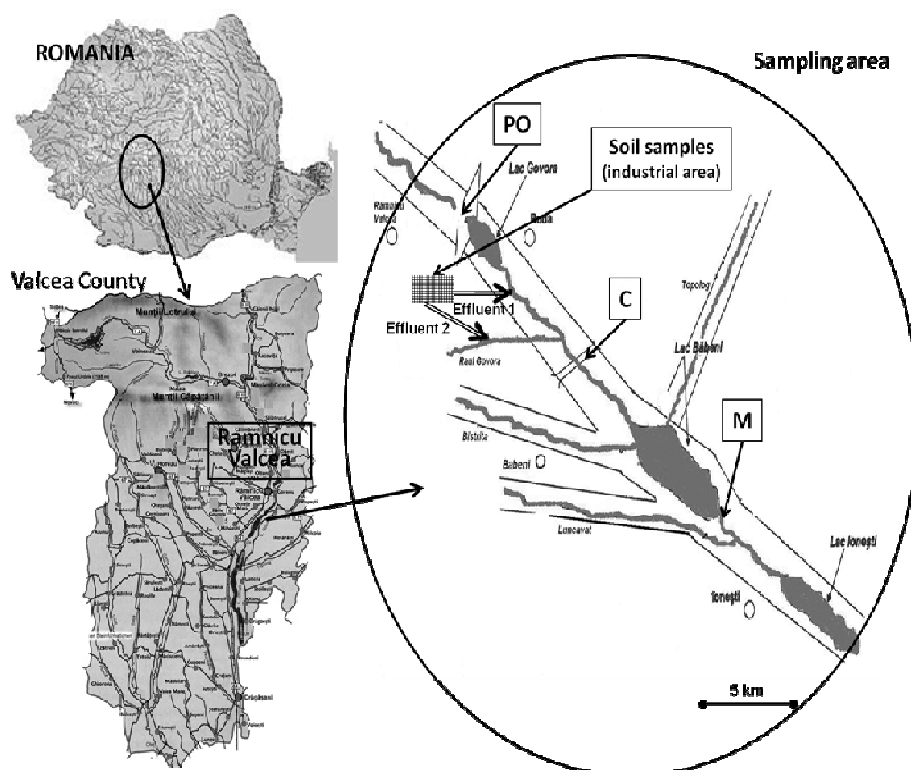

Figure 2. Location of Ramnicu Valcea, its industrial area, water/sediment sampling collection points (PO, C and M) [Iordache M., et al., 2014]

3. RESULTS AND DISCUSSION

3.1. The transfer of organochlorine compounds in the environment in the Babeni-Marcea and Cremenari sections from Olt River

The mathematical model was developed for analysis of organochlorine substances (1, 2-dichloroethane, trichlorethylene, perchlorethylene and 1, 2, 4-trichlorobenzene). In order to compare the results of the modelling, we used the experimental values presented in Table 2 and 3. The values of the modelling are presented in Tables 4-11.

Starting from the measured values for these pollutants in environmental factor "water" was achieved transfer of these hazardous pollutants modelling environments "sediment", "biota" and "air". Of course, to validate this model were considered values obtained for "sediment", as these types of evidence have been worked as a real samples in the laboratory. The following are presented point for each sampling point was studied, the results and conclusions highlighted. Biota are approximate quantity of 1 part / m^3 = 7.83 x 1 million 107/106 = 78.3

Table 2. The content of organochlorine compounds in water of the Olt River, (µg/L)

Sample designation	The period	Quality indicators analysed			
		1,2-DCE	1,1,2-TCE	PCE	1,2,4 TCB
C	Mai 2013	0.500	<0.05*	<0.05*	<0.002*
	August 2013	0.520	<0.05*	<0.05*	<0.002*
	March 2014	2.990	0.850	4.900	<0.002*
	August 2014	1.950	0.740	2.400	<0.002*
M	Mai 2013	0.200	<0.05*	<0.05*	<0.002*
	August 2013	0.240	<0.05*	<0.05*	<0.002*
	March 2014	2.560	<0.05*	1.900	<0.002*
	August 2014	1.020	<0.05*	0.780	<0.002*

* The detection limit of the method

Table 3. The content of organochlorine compounds in sediments of the Olt River, (mg/kg d.w.)

Sample designation	The period	Quality indicators analysed			
		1,2-DCE	1,1,2-TCE	PCE	1,2,4 TCB
C	Mai 2013	<0.05*	<0.05*	<0.05*	<0.002*
	August 2013	<0.05*	<0.05*	<0.05*	<0.002*
	March 2014	<0.05*	<0.05*	<0.05*	<0.002*
	August 2014	<0.05*	<0.05*	<0.05*	<0.002*
M	Mai 2013	<0.05*	<0.05*	<0.05*	<0.002*
	August 2013	<0.05*	<0.05*	<0.05*	<0.002*
	March 2014	<0.05*	<0.05*	<0.05*	<0.002*
	August 2014	<0.05*	<0.05*	<0.05*	<0.002*

* The detection limit of the method

3.2. Transfer of organochlorine substances in Section Băbeni Marcea

3.2.1. Transfer of 1, 2-dichloroethane

The values obtained for the environmental "sediment" in the modelling transfer of 1,2-dichloroethane in water was very similar to those determined experimentally for measurement campaigns in 2013: ex. 0.052 mg/kg and 0.062 mg/kg to the level of 0.05 mg/kg (the detection limit of the method).

The values obtained for the environmental "sediment" in the modelling transfer of 1,2-dichloroethane in water was slightly higher than those determined experimentally for the 2014 measurement campaigns (eg. 0.662 mg/kg and 0.264 mg/kg) compared to the value 0.05 mg/kg (the detection limit of the method). However, these shapes with a good enough uncertainty levels in this type of substance in this sediment sampling, indicating an average concentration level of <0.05 mg/kg.

From the modeled values was clearly observed tendency of this pollutant transfer the component "air" but observed that a large amount of the component is taken "biota" in averages approx. 0.3 mg/kg for 2013 and 2 mg/kg for 2014, which corroborated the degree of toxicity of this compound and should be a warning about the level of environment.

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Table 4. Transfer of 1, 2-dichloroethane in Babeni – Marcea (M) section

Concentrations determined (M)	Prognosis in air ng/m3	The measured in water (M) µg/L	Prognosis in sediment mg/kg	Prognosis in biota mg/kg	The measured in sediment (M)	The measured in sediment (C)
May 2013	14.679	0.200	0.052	0.271	<0.05	<0.05
August 2013	17.615	0.240	0.062	0.325	<0.05	<0.05
March 2014	187.891	2.560	0.662	3.463	<0.05	<0.05
August 2014	74.863	1.020	0.264	1.380	<0.05	<0.05
	References	Table 1			Table 2	Table 2

3.2.2. Transfer of Trichlorethylene

The values obtained for the environmental "sediment" in the modelling transfer of trichlorethylene in water are close to those determined experimentally for measurement campaigns in 2013: ex. 0.121 mg/kg to the level of 0.05 mg/kg (the detection limit of the method).

Table 5. Transfer of trichloroethylene in Babeni – Marcea (M) section

Concentrations determined (M)	Prognosis in air ng/m3	The measured in water (M) µg/L	Prognosis in sediment mg/kg	Prognosis in biota mg/kg	The measured in sediment (M)	The measured in sediment (C)
May 2013	49.911	<0.05	0.121	0.631	<0.05	<0.05
August 2013	49.911	<0.05	0.121	0.631	<0.05	<0.05
March 2014	509.091	0.510	1.231	6.439	<0.05	<0.05
August 2014	349.376	0.350	0.845	4.419	<0.05	<0.05
	References	Table 1			Table 2	Table 2

The values obtained for the environmental "sediment" in the modeling transfer of trichlorethylene in water are slightly higher than those determined experimentally by measuring campaigns in 2014 (ex. 1.231 mg/kg and 0.845 mg/kg compared to the value of 0.05 mg/kg (the detection limit of the method)). However, these shapes with a good enough uncertainty levels in this type of substance in this sediment sampling, indicating an average concentration level of <0.05 mg/kg.

From the modelled values is clearly observed tendency of this pollutant transfer in section "air" but observed that a significant amount is taken from section "biota" in averages approx. 0.6 mg/kg for 2013 and 5 mg/kg for 2014, which corroborated the degree of toxicity of this compound and should be a warning about the level of environmental pollution in the area.

3.2.3. Transfer of Perchlorethylene

The values obtained for the environment al "sediment" in the modelling transfer of perchlorethylene in water are close to those determined experimentally for measurement campaigns in 2013: ex. 0.215 mg/kg to the level of 0.05 mg/kg (the detection limit of the method).

The values obtained for the environmental "sediment" in the modelling transfer perchlorethylene in water are higher than those determined experimentally by measuring campaigns in 2014 (ex. 8.158 mg/kg and 3.349 mg/kg compared to the value of 0.05 mg/kg (the detection limit of the method)). However, these shapes with a good enough uncertainty levels in this type of substance in this sediment sampling, indicating an average concentration level of <0.05 mg/kg.

From the modelled values is observed that a large amount is taken from component "biota" in averages approx. 1.12 mg/kg for 2013 and 30.0 mg/kg for 2014, which corroborated the degree of toxicity of this compound and should be a warning about the level of environmental pollution in the area.

Table 6. Transfer of perchlorethylene in Babeni – Marcea (M) section

Concentrations determined (M)	Prognosis in air ng/m3	The measured in water (M) µg/L	Prognosis in sediment mg/kg	Prognosis in biota mg/kg	The measured in sediment (M)	The measured in sediment (C)
May 2013	0.019	<0.05	0.215	1.123	<0.05	<0.05
August 2013	0.019	<0.05	0.215	1.123	<0.05	<0.05
March 2014	0.706	1.900	8.158	42.657	<0.05	<0.05
August 2014	0.290	0.780	3.349	17.512	<0.05	<0.05
	References	Table 1			Table 2	Table 2

3.2.4. Transfer of 1, 2, 4-trichlorobenzene

The values obtained for the environmental "sediment" in the modelling transfer of 1,2,4-trichlorobenzene in water are close to those determined experimentally for measurement campaigns in 2013 and 2014: ex. 0.188 mg/kg to the value of 0.002 mg/kg (the detection limit of the method).

From the modelled values is observed that a large amount is taken from section "biota" in averages approx. 1 mg/kg in 2013 and 2014, which corroborated the degree of toxicity of this compound and should be a warning about the level of environmental pollution in the area.

Table 7. Transfer of 1, 2, 4 - trichlorobenzene in Babeni – Marcea (M) section

Concentrations determined (M)	Prognosis in air ng/m3	The measured in water (M) µg/L	Prognosis in sediment mg/kg	Prognosis in biota mg/kg	The measured in sediment (M)	The measured in sediment (C)
May 2013	0.000	0.002	0.188	0.982	<0.002	<0.002
August 2013	0.000	0.002	0.188	0.982	<0.002	<0.002
March 2014	0.000	0.002	0.188	0.982	<0.002	<0.002
August 2014	0.000	0.002	0.188	0.982	<0.002	<0.002
	References	Table 1			Table 2	Table 2

3.3. Transfer of organochlorine substances in Section Cremenari

3.3.1. Transfer of 1, 2 – dichloroethane

The values obtained for the environmental "sediment" in the modelling transfer of 1,2-dichloroethane in water are very similar to those determined experimentally for measurement campaigns in 2013: ex. 0.129 mg/kg and 0.135 mg/kg to the level of 0.05 mg/kg (the detection limit of the method).

The values obtained for the environmental "sediment" in the modelling transfer of 1,2-dichloroethane in water are slightly higher than those determined experimentally for the 2014 measurement campaigns (eg. 0.773 mg/kg and 0.504 mg/kg to value of 0.05 mg/kg (the detection limit of the method)). However, these shapes with a good enough uncertainty levels in this type of substance in this sediment sampling, indicating an average concentration level of <0.05 mg/kg.

From the modelled values is clearly observed tendency of this pollutant transfer in section "air" but observed that a significant amount is taken from section "biota" in averages approx. 0.7 mg/kg for 2013 and 3 mg/kg for 2014.

Table 8. Transfer of 1, 2 - dichloroethane in Cremenari (C) section

Concentrations determined (C)	Prognosis in air ng/m3	The measured in water (M) µg/L	Prognosis in sediment mg/kg	Prognosis in biota mg/kg	The measured in sediment (C)	The measured in sediment (M)
May 2013	36.697	0.500	0.129	0.676	<0.05	<0.05
August 2013	38.165	0.520	0.135	0.703	<0.05	<0.05
March 2014	219.450	2.990	0.773	4.044	<0.05	<0.05
August 2014	143.120	1.950	0.504	2.638	<0.05	<0.05
	References	Table 1			Table 2	Table 2

3.3.2. Transfer of Trichlorethylene

The values obtained for the environmental "sediment" in the modelling transfer of trichlorethylene in water are close to those determined experimentally for measurement campaigns in 2013: ex. 0.121 mg/kg to the level of 0.05 mg/kg (the detection limit of the method).

The values obtained for the environmental "sediment" in the modelling transfer of trichlorethylene in water are slightly higher than those determined experimentally by measuring campaigns in 2014 (ex. 2.052 mg/kg and 1.787 mg/kg compared to the value of 0.05 mg/kg (the detection limit of the method)). However, these shapes with a good enough uncertainty levels in this type of substance in this sediment sampling, indicating an average concentration level of <0.05 mg/kg.

From the modelled values is clearly observed tendency of this pollutant transfer in section "air" but observed that a significant amount is taken from section "biota" in averages approx. 0.6 mg/kg for 2013 and 9 mg/kg for 2014.

Table 9. Transfer of trichloroethylene in Cremenari (C) section

Concentrations determined (C)	Prognosis in air ng/m3	The measured in water (M) µg/L	Prognosis in sediment mg/kg	Prognosis in biota mg/kg	The measured in sediment (C)	The measured in sediment (M)
May 2013	49.911	<0.05	0.121	0.631	<0.05	<0.05
August 2013	49.911	<0.05	0.121	0.631	<0.05	<0.05
March 2014	848.486	0.850	2.052	10.731	<0.05	<0.05
August 2014	738.682	0.740	1.787	9.342	<0.05	<0.05
	References	Table 1			Table 2	Table 2

3.3.3. Transfer of Perchlorethylene

The values obtained for the environmental "sediment" in the modelling transfer of water perchlorethylene are close to those determined experimentally for measurement campaigns in 2013: ex. 0.215 mg/kg to the level of 0.05 mg/kg (the detection limit of the method).

The values obtained for the environmental "sediment" in the modelling transfer perchlorethylene in water are higher than those determined experimentally by measuring campaigns in 2014 (i.e. 21.040 mg/kg and 10.305 mg/kg compared to the value of 0.05 mg/kg (the detection limit of the method)). However, these shapes with a good enough uncertainty levels in this type of substance in this sediment sampling, indicating an average concentration level of <0.05 mg/kg.

From the modelled values is observed that a large amount is taken from section "biota" in averages approx. 1.12 mg/kg for 2013 and 80.0 mg/kg for 2014.

Table 10. Transfer of perchlorethylene in Cremenari (C) section

Concentrations determined (C)	Prognosis in air ng/m3	The measured in water (M) µg/L	Prognosis in sediment mg/kg	Prognosis in biota mg/kg	The measured in sediment (C)	The measured in sediment (M)
May 2013	0.002	<0.05	0.215	1.123	<0.05	<0.05
August 2013	0.002	<0.05	0.215	1.123	<0.05	<0.05
March 2014	0.203	4.900	21.040	110.011	<0.05	<0.05
August 2014	0.099	2.400	10.305	53.883	<0.05	<0.05
	References	Table 1			Table 2	Table 2

3.3.4. Transfer of 1, 2, 4-trichlorobenzene

The values obtained for the environmental "sediment" of 1,2,4-trichlorobenzene transfer the modelling of water are close to those determined experimentally for measurement campaigns in 2013 and 2014: ex. 0.188 mg/kg to the value of 0.002 mg/kg (the detection limit of the method).

From the modelled values is observed that a large amount is taken from section "biota" in averages approx. 1 mg/kg and 2013 and for 2014, which corroborated the degree of toxicity of this compound and should be a warning about the level of environmental pollution in the area.

Table 11. Transfer of 1, 2, 4- trichlorobenzene in Cremenari (C) section

Concentrations determined (C)	Prognosis in air ng/m3	The measured in water (M) µg/L	Prognosis in sediment mg/kg	Prognosis in biota mg/kg	The measured in sediment (C)	The measured in sediment (M)
May 2013	0.000	0.002	0.188	0.982	<0.002	<0.002
August 2013	0.000	0.002	0.188	0.982	<0.002	<0.002
March 2014	0.000	0.002	0.188	0.982	<0.002	<0.002
August 2014	0.000	0.002	0.188	0.982	<0.002	<0.002
	References	Table 1			Table 2	Table 2

4. CONCLUSIONS

The analysis results can synthesize modelling study organochlorine following general conclusions:

- model based on "fugacity" realistic indicative values generated applied to environmental compartments of interest respectively, air, sediment, biota;
- modelled values obtained for section "sediment" were comparable and compatible with the values of the laboratory analytical determinations;
- uncertainty modelled values obtained should be read in conjunction with the following factors: (1) for simplicity and applicability as faster and easier model applied not made detailed calculations to be included in river flow, so that the dilution factor may vary from year to year, depending on annual meteorological factors; (2) that approximating model made by the volume of Lake Babeni, we believe that water is stationary (not running) for a sufficiently high so as to achieve equilibrium phase transfer modelling based on "fugacity" pollutant between "compartments", which has also generated the degree of error in the values obtained modelled;
- modelled values obtained for section "sediment" are comparable and compatible with the values obtained by analytical measurements, which provides a quick indication of the respective pollutant pollution environmental compartment studied;
- modelling revealed clear trend the transfer of component "air" of these pollutants are known fact that volatile compounds;
- however, based on modelling was observed a significant transfer of these pollutants in the factor "biota" in amounts which may generate medium and long term risk to human health by taking in the food chain, which at first sight and a first risk assessment made by these pollutants for local residents can go unnoticed;
- although the degree of error values obtained model was slightly increased due consideration as stationary and no water flowing pattern transfer application proves a useful tool for estimating pollution levels quickly analyse environmental pollutants without costly development of analytical determinations in terms of time and money.

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