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TRICLOCARBAN PARTITION COEFFICIENTS IN WATERS WITH DIFFERENT COMPOSITIONS

Ion ION[1], Roxana CORNOIU[1], Tudorita TOFAN[1], Alina Catrinel ION[1]

Triclocarban (TCC) is a hydrophobic organic compound used in personal care products as a bactericidal reagent, that poses ecological risks due to inadequate wastewater treatment. This study investigates the effects of water's chemical composition on TCC solubility in natural water environment. Its K_{ow} *and* K_{salt}*, which reflect TCC partition coefficients, are influenced by physical and chemical parameters, such temperature, pH and the total concentration of salts in the aqueous media. The results offer insights for future TCC removal research from natural waters.*

Keywords: triclocarban, natural water, octanol – water partition coefficient, solubility

1. Introduction

Organic and inorganic chemicals are discharged in aquatic media mostly through wastewaters, treated or not treated [1]. The emerging pollutants remain in water and risk health to several organisms even at very low concentrations can appear [2].

Triclocarban (TCC) is an organic antibacterial substance used in personal care products, with unpleasant endocrine effects and further antibacterial resistance, depending on its concentrations in the environment. An important source of TCC in natural waters is an insufficient removal in the treatment plants, or an inefficient treatment of wastewater, contaminating in this way the water, the sediments and the aquatic life [3]. Water solubility, the octanol-water partition coefficient K_{ow} and the salt distribution constant K_{salt} are important parameters which determine the environmental concentrations, or how the substance leaches in soil or moves with the runoff.

Solubility data offer information about dissolution in water and in tissues, absorption and adsorption processes and adsorption rates.

K_{ow} (the octanol-water partition coefficient) expresses the ratio of concentration at equilibrium of a dissolved substance between octanol and water at constant temperature). Correlated with its solubility in water (S), it emphasizes the risk assessment characteristics based on the environmental concentrations of TCC and the ecological health risks. K_{ow} has an important significance in living organisms,

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[1] National University of Science and Technology POLITEHNICA Bucharest, Romania, e-mail: alina.ion@upb.ro

because it reflects the membrane water:lipid barrier and further, its bioaccumulation in organic tissues. Octanol is similar to lipids in living organisms having the same carbon to oxygen ratio. These two indicators make possible the estimation of amount of TCC in aquatic environment available for microbial degradation and bioaccumulation.

In inorganic electrolyte solutions the solubility of organic compounds modifies, based on their polarities, inorganic salts increasing water polarity and expelling the nonpolar solute. This effect is emphasized by the Setschenow constant: $\log S/S_0 = K_{salt}C_{salt}$, where S and S_0 refer to the solubility of the organic compound in inorganic salts solution and in water, C_{salt} refers to the molar concentration of electrolyte and K_{salt} is the Setschenow constant [4].

Usually, the distribution of organic compounds in natural aqueous matrices mainly depends on the chemical matrix of the natural water, or to temporal changes [5]. The dermal exposure to triclocarban contained in various solvents such as acetone, acetonitrile, DMF or cleanser was studied and quantified for humans or rats, because it seems that the rat skin is between 4 to 7 times more permeable to triclocarban than human skin. In humans, it was estimated that without a rinsing step, about 7 %, applied triclocarban dissolved in acetone was absorbed and systemically available. In a typical rinse-off scenario, mimicked by a showering study with human subjects using triclocarban containing bar soap, about 0.39% triclocarban of the total applied dose was available. This study was necessary on the one hand due its use as preservative in personal care products. In vitro studies with natural and in purpose blessed human skin, models suggested that blessed human skin was about 2 times more permeable than the not-blessed one. On the other hand, the dependence of triclocarban solubility on the concentration of inorganic salts from the aqueous media influences its bioavailability in connection with the environment [6].

Different values for the water solubility and K_{ow} of TCC were found in literature [7,8], log K_{ow} values for triclocarban ranging between 4.2 to 6.0 [9]. Several properties of organic hydrophobic compounds might be included in estimating this characteristic in different solvents like: structural fragments, solvation properties, area of the polar surface, lipophilicity, melting point, type of heteroatoms, double bonds, hydrogen bonds [10]. pK_a of the studied compounds and the pH of solvation medium are also taken into consideration [11]. In what concerns the K_{salt} values, there are not reported in the literature till this moment, based on our knowledge.

The purpose of this study is to contribute at the database required for TCC risk assessment in water bodies, being known its tendency to bioaccumulate. The octanol-water partition coefficient of TCC was determined in natural waters with various chemical compositions, based on [12], in order to see how the chemical matrix of the aqueous solution influences the distribution of triclocarban in binary

systems. The values were obtained based on of TCC solubility determined in the same matrices by Higuchi's Facilitated Dissolution Method (FDM), that suggests the add of a small volume of a water-immiscible solvent to help the decrease of contact time for compounds with slow dissolution rates [13].
The dependence of K_{salt} for triclocarban in NaCl solutions and then in some natural waters with different mineralization, of the octanol-water partition coefficient K_{ow} of triclocarban was calculated.

2. Materials and Methods

2.1. Materials

The following substances were used: triclocarban (TCC), (99% purity), Fluka/Sigma-Aldrich Chemical, Germany; 0.1 mol/L sodium chloride (0.1 N), Scharlau; acetonitrile HPLC grade, Merck; 1-octanol HPLC grade Merck, PTFE 0.22 µm syringe filters; samples of various types of waters. Ultrapure water was provided by a Direct Q3 UV system, Merck, Germany.

2.2. Methods

The experiments over TCC behavior in aqueous systems were performed in order to determine its octanol - water partition coefficients and its solubility in pure water, in several NaCl solutions and in natural waters with different compositions, with a small volume in each (1%) of 1-octanol. From stock solutions of TCC in octanol, or acetonitrile, depending on the type of experiment, there were prepared the working solutions of TCC and the following influences were studied over the TCC solubility, K_{ow} and K_{salt} derived from K_{ow}: temperature (5 - 40°C); contact time (at 25°C); pH (at 25°C); ionic strength (0.01 – 0.15 mol/L NaCl; electric conductivity which outlines the total amount of minerals in the natural mineral water.

2.3. HPLC method

The measurements were performed with a chromatograph Agilent 1100 HPLC and Chemstation software for data analysis. Chromatographic parameters of the method are: the volume of injection: 25 µL; analysis time: 10 min; column temperature: 25°C; stationary phase: C18, 3.5 µm, 100 × 4.6 mm id; flow rate: 1 ml/min, isocratic conditions; the composition of the mobile phase acetonitrile: water mixture (80:20 v/v). TCC readings were established at $\lambda = 265$ nm by using the UV-Vis detector. Based on external standard calibration method on concentration ranges between: 1 µg/L ÷ 100 µg/L and 10 µg/L ÷ 400 µg/L TCC concentrations were determined. These concentration ranges were chosen for validating this method in aqueous samples with different matrices which influence the equilibrium concentration of TCC.

2.4. Characterization of the aqueous samples

The aqueous samples used for this study were analyzed, in what concerns pH, electrical conductivity (e.c.), cations (Na^+, K^+, $Ca^{2+,}$ Mg^{2+}) and anions (Cl^-, NO_3^-, SO_4^{2-}) concentrations, being presented in Table 1. Several techniques were used in this purpose, such as: electrochemical, volumetric, gravimetric and inductively coupled plasma optical emission spectrometry (ICP-OES) [14, 15, 16].

Table 1

Physical-chemical characterization of natural waters

pH at 21.5 °C	C.e. µS/cm	Cl^- mg/L	SO_4^{2-} mg/L	HCO_3^- mg/L	Ca^{2+} mg/L	Mg^{2+} mg/L	Na^+ mg/L	Fe_{tot} mg/L
5.9	1100	8.08	0.90	673	86.7	19.40	144	6.42
6.0	904	6.74	9.22	793	162	30.10	69.60	7.40
7.3	290	4.00	8.00	190	47.00	10.00	0.75	1.00
7.1	500	5.00	18.00	320	50.00	45.00	5.00	2.00
7.0	5	0.05	0.00	0.00	0.00	0.00	0.05	0.00

2.5. TCC solubility experiments

The water solubility of TCC was analyzed using a modified EPA procedure, column elution method (USEPA, 1996a) [17], combined with Higuchi's facilitated dissolution method (FDM), which is dedicated to the compounds with water solubility less than 10 mgL^{-1}. TCC is dissolved in acetonitrile with 0.25 % v/v 1-octanol, deposed onto glass beads, and dried. Approx. 2-3g of loaded beads are introduced into a glass column of 20 cm, representing 1/8 from the total volume, the rest being occupied by ultrapure water, aqueous solutions with different concentrations of NaCl and natural waters with different compositions, used in these experiments, in each 1% 1-octanol being added. (Table 1) The variation of the temperature is assured by a thermostatic column during experiments. The time of contact is of 5 hours, samples being collected and analyzed each 30 minutes. The equilibrium was considered established when five successive samples have concentrations with values differing less than 30%.

2.6. *Octanol-water partition coefficient (K_{ow}) of TCC*

The K_{ow} was considered as the ratio of concentrations of a dissolved substance, at equilibrium, in octanol:water. It was obtained based on EPA Guidelines for partition coefficient n-octanol/water [18]. Octanol and ultrapure water were saturated at each experimental temperature. An initial concentration of TCC solution was prepared by dissolving 10 mg of organic compound in 150 mL of octanol, then certain volumes were mixed with ultrapure water, NaCl aqueous solutions with different concentrations and natural mineral waters with different matrices to obtain the experimental volume ratios, of 1:1, 1:1.5 and 1:2. TCC solution in octanol as solvent and waters with different chemical compositions were combined in centrifuge tubes of 30 mL and centrifuged for 5 minutes for separation, then 1 mL of aliquots were taken for analysis. Each ratio was run in triplicate, log K_{ow} value being obtained from average results with a difference between them less than $\pm$0.5.

2.7. Salt effect parameter, Setschenow constant (K_{salt})

Our objective was to determine the Setschenow constant K_{salt}, in NaCl solutions with different concentrations and natural mineral waters, from experimentally obtained solubilities and octanol-water partition coefficients K_{ow} of triclocarban, experimentally determined, based on the correlation between the logarithmic value of K_{ow} and the Setschenow constant: $K_{salt} = 0.039\log K_{ow} + 0.117$. If K_{salt} value is positive, then the present salts in the aqueous solution will decrease triclocarban solubility in water, facilitating its distribution in existing sediments from environmental matrices.

3. Results and Discussions

3.1. TCC water solubility, K_{ow} and K_{salt}

TCC solubility was measured, three times each, in ultrapure and in different water electrolytes (NaCl or more complex) solutions. K_{ow} was measured and calculated as logarithmic value, in the partitioning test. It was observed that by using Higuchi’s method, the necessary time for attaining equilibrium solubility was two hours. The obtained values for the solubility and K_{ow} show a relationship between these parameters, the importance of obtaining data by standardized methodologies becoming more and more clear. There are several K_{ow}/solubility relationships available for the calculations, like linear free-energy ones (LFERs) and EPI Suite. LFER can be developed by studying many substances like that of interest and the regression coefficient being an indicator of good predictability. EPI Suite programs (ECOSAR, KOWWIN, WATERNT, WSKOWWIN) can also be used for estimating the values of solubility and K_{ow}, all of them with some mismatches [19]. The bias in predicted TCC solubilities and log K_{ow}, based on the estimation program, confirm the importance of correctly obtained experimental physical-chemical parameters. Only WSKOWWIN allows manual entry of the physicochemical parameters [20]. These two parameters, S and log K_{ow}, that were measured, are very important in estimating the environmental health risk of organic pollutants. There are also several formulas to quantitatively determine the effect of the salt present in solution on the solubility of organic compounds, such as: electrostatic Debye MacAulay theory [21], or that of Xie and Mackay [22] which uses several parameters to determine K_{salt}, with debatable results.

The Setschnow constant K_{salt} of an organic compound in aqueous salt solutions was shown to be related by a linear correlation to the logarithmic value of octanol-water partition coefficient K_{ow}, based on the Yalkowsky equation: $K_{salt} = A\log K_{ow} + B$, where A and B are constants [23].

3.2. Effect of temperature on solubility, K_{ow} and K_{salt} of triclocarban in synthetic solutions

How the temperature influences these physical-chemical parameters was evaluated in ultrapure water with a concentration of NaCl of 0.01 M, at temperatures in the range 5 and 35-40°C (represented in degree Kelvin in the graph), this range of temperatures characterizing all the seasons of the year. The averaged results of three replicates each, for K_{salt} determination are presented in Figure 1.

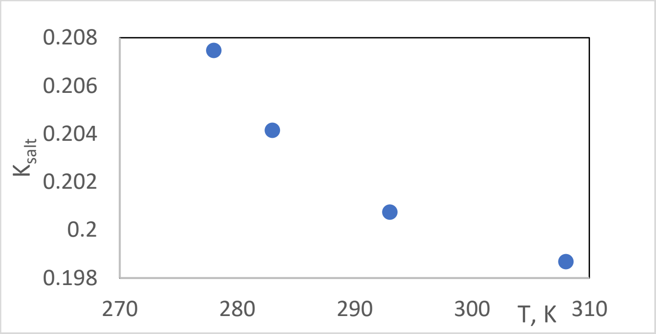

Fig. 1. Influence of the temperature over K_{salt} of triclocarban in aqueous solution

Based on these results, the calculated K_{salt} values from experimentally determined log K_{ow} values decrease by increasing temperature. This trend can be due to the values of octanol-water distribution coefficient of TCC, which express a lower content of TCC in water. Higher temperatures lead to a better solubility of TCC in water (meaning more TCC molecules being dissolved).

Table 2

Effect of variation of the temperature over the triclocarban solubility in aqueous media

Temperature, °C	**S_{TCC} concentration, mg/L**	**log K_{ow}**	**K_{salt}**
5	0.112 (±0.002)	2.3198	0.2074
10	0.122 (±0.001)	2.2344	0.2041
20	0.143 (±0.002)	2.1473	0.2007
35	0.154 (±0.002)	2.0944	0.1986

The values from the table indicate an increase of triclocarban solubility by temperature, in connection with the variation of the Gibbs free energy: $\Delta G=-RT\ln K$, with ΔG - the Gibbs free energy from the transfer reaction, R - the ideal gas constant (J/mol·K) and T - temperature (K). The value of partition constant K is reduced while S increases, based on the correlation: $\ln S_{TCC}$ (molL^{-1}) = $-\Delta_{sol}H/RT + C$; logS (mol/L) = 0.79-0.85 log K-0.0073MW.

3.3. *Effect of pH on triclocarban aqueous solubility*

pH is another factor that might influence the K_{ow} and solubility in aqueous matrices. The pH of ultrapure water, with a small concentration of 0.01 M NaCl was adjusted by using 0.1M HCl, or NaOH solution and its effect was studied in a range of pH between 5 and 12, in three replicates and the results are presented in Figure 2 and Table 3.

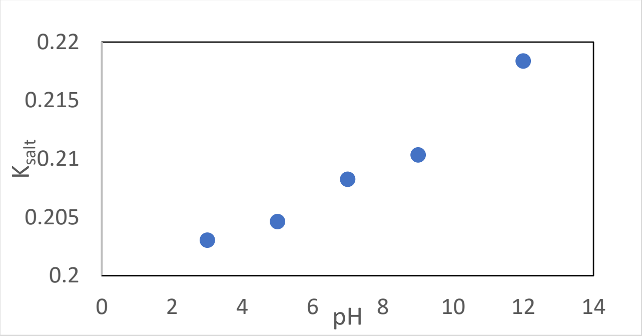

Fig. 2. Effect of the variation of pH over K_{salt} values of triclocarban TCC, at 25 ^{0}C

The data above show that K_{salt} slightly varies in the pH range between 3 and 12. TCC is a trichloro carbanilide with a pK_a around 12 and triclocarban dissociates at pH values higher than this value, where the TCC ionized form predominates and the solubility is influenced by pH value.

Table 3

Effect of pH over TCC logKow correlated with K_{salt} values, at 25°C

pH	**TCC concentration, mg/L**	**log Kow**	**K_{salt}**
3	0.13	2.2063	0.2030
5	0.120 (±0.004)	2.2470	0.2046
7	0.100 (±0.004)	2.3397	0.2082
9	0.090 (±0.002)	2.3933	0.2103
12	0.060 (±0.002)	2.5995	0.2183

The results presented in the table above showed that the logarithmic values of K_{ow} slightly modified before a pH value around 12, but these increase above it. A possible explanation might be that till approx. pH 12, the values are within the pK_a range of TCC, below pH 12, TCC existing in its neutral form and K_{ow} presenting usually higher values if the organic compound is in its neutral form. The positive values of K_{salt} indicate a salting-out effect, so triclocarban solubility will decrease in water with increased concentrations of inorganic salts.

3.4. Influence of NaCl concentration in aqueous samples on the solubility of triclocarban

The experiments were done in NaCl aqueous solutions of concentrations between 0.01 - 0.15 mol/L at 25°C. Averaged results of repeated measurements are presented in Figure 3 and Table 4.

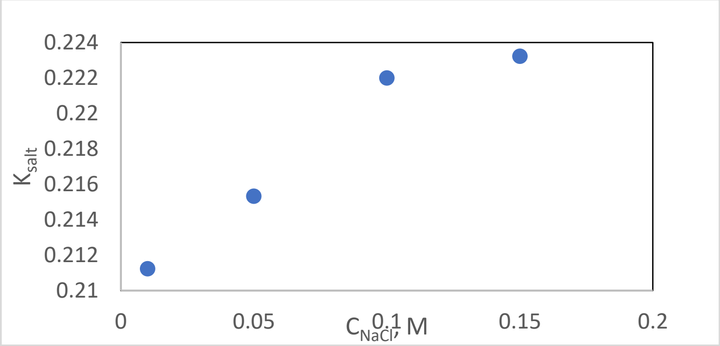

Fig. 3. Effect of the variation of NaCl concentration over log K_{salt} values of triclocarban TCC, at 25 ^{0}C

The value of ionic strength of the aqueous solution affects the partition of organic compounds between the organic and the aqueous phases. It can be observed that the relationship between ionic strength of the aqueous solution shows that an increase of ionic strength produces an increase of the partition in the organic phase of TCC (the salting-out effect). At higher concentrations of NaCl (>0.2 M), polar molecules might have electrostatic interactions with the ions from the aqueous solution, the values of log K_{ow} no longer varying so much. The obtained curve fits a polynomial dependence, with a value of R^2 of 0.9758, supporting the idea of a higher bioaccumulation of TCC in the aquatic organisms at higher values of ionic strength of the aqueous solutions. The data concerning the TCC concentrations in aqueous samples with different compositions is also supported by Weise et al. [24].

Table 4

Ionic strength influence over the values of triclocarban solubility, at 25°C

NaCl, mol/L	TCC, mg/L	log K_{ow}	K_{salt}
0.01	0.078 (±0.002)	2.4165	0.2112
0.05	0.067 (±0.002)	2.5211	0.2153
0.1	0.055 (±0.002)	2.6923	0.2219
0.15	0.0456 (±0.002)	2.7237	0.2232

It is observed a decrease of the TCC concentration by gradually increasing ionic strength. The obtained data reflects the influence of the salt concentration over the solubility of organic compounds. At higher values of ionic strength, TCC will predominate into the organic phase in an aqueous: organic solvent mixture.

3.5. *Effect of the total ionic salt concentration of natural water samples on triclocarban solubility*

The study of the effect of natural water's composition on the TCC concentration was carried out in five natural water samples with different compositions, mainly based on the presence of Na^+ and Cl^- ions and in ultrapure water (UPW). A set of five samples for each water was performed at 5, 25 and 35-40 °C in an electrical incubator (120 rpm). Results are presented below in Figure 5 and Table 6.

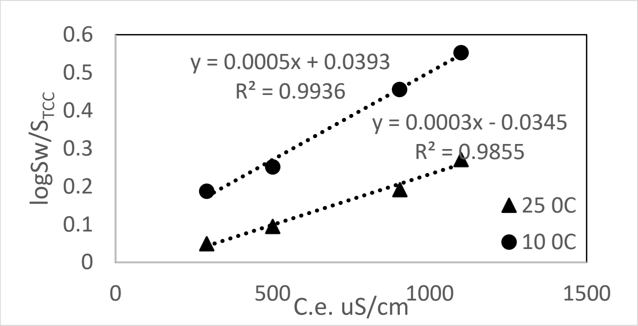

Fig. 5. Effect of the total ionic salt concentration of water samples over the solubility of TCC in several aqueous matrices, at 10 and 25 ^{0}C

As it can be observed from Figure 5, the empirical Setschenow constant $\log(S_w/S) = K_{salt}xC_{salt}$ gives a satisfactory description of the relationship between the salt concentration in aqueous solution and the solubility of the organic solute, displaying the salting effect. At 10 ^{0}C a better correlation is observed, the slope value being closer to the K_{salt} values experimentally determined from K_{ow} ones. The ratio S_w/S is determined taking into account the solubility of TCC in the water sample with the electric conductivity of 5 µS/cm, as reference.

Table 6

Effect of the total ionic salt concentration of natural water samples on triclocarban aqueous solubility

pH at 21.5 °C	C.e. µS/cm	Cl^-, mg/L	Na^+, mg/L	T,^{0}C	TCC,mg/L
5.9	1100	8.08	144	5 25 35	0.010 0.035 0.040
6.0	904	6.74	69.60	5 25 35	0.035 0.070 0.076
7.3	290	4.00	0.75	5 25 35	0.065 0.100 0.110
7.1	500	5.00	5.00	5 25 35	0.056 0.090 0.098
7.0	0.05	0.05	0.05	5 25 35	0.104 0.112 0.120

In solution, energy is supplied to reduce the cohesion forces of the solute and of the solvent and to generate the space for the solute molecules in solution. All these processes contribute to the organic compound solubility in any solvent and these will vary based on its chemical composition. This will be mainly influenced by the van der Waals and Lewis acid-base interactions.

Table 7

Values of TCC S and Kow obtained in the literature for several aqueous matrices

Solubility of TCC, mg/L	Log Kow	Observations	References
0.178	4.40	In environmental aqueous matrix	[25]
1.60	-	Aquatic environment	[26]
-	4.65-4.90	Several aqueous matrices	[27]

There are several already reported results for found concentrations of TCC in aqueous matrices which are presented in the table above (Table 7), but no K_{ow} values, considering binary systems water:organic solvents in which TCC is soluble. Partition coefficients calculated in appropriate solvents might be useful in several laboratory experiments, as well as in technologies concerning wastewaters treatments. The obtained values might also be important in studying lipophilic organic compounds and their behavior in contact with living organisms.

4. Conclusions

In this study, how several characteristics of natural waters (temperature, pH, ionic strength, and salts concentration) influence the K_{ow}, solubility and K_{salt} of TCC, was presented.

From the obtained data it was observed that all physical-chemical parameters that describe the TCC behavior in aqueous matrices are influenced by temperature, the values of the solubility increasing by temperature from 0.112 to 0.143, between 5 and 35-40°C. By increasing ionic strength, the solubility of TCC decreases from 0.0780 to 0.0456. It was observed that pH slightly affects TCC concentration in synthetic aqueous solutions. The obtained results suggest links that are established between log K_{ow}, K_{salt} and environmental aqueous matrices which can offer important information about TCC solubility and distribution in these media.

The composition of waters where TCC might appear as an environmental hydrophobic contaminant is mainly important for its distribution in these matrices, many industrial processes producing effluents containing important concentrations of electrolytes which change the effect of hydrophobic contaminants both in treatment stations and in receiving waters.

These preliminary results could be the basis for future ones, in complex aqueous matrices used for correlations of triclocarban solubility with their composition, in order to estimate the bioconcentration and bioaccumulation of TCC in natural waters and its further influence over the aquatic life and also as good predictors for removal efficiency from these matrices.

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