

# A Fugacity Based Model for the Assessment of Pollutant Dynamic Evolution of VOCS and BTEX in the Olt River Basin (Romania)

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*An important tributary of the Danube River, the Olt River, was characterized in its middle and lower catchment in terms of volatile organic compounds (1,2 -dichloroethane and perchlorethylene) and volatile aromatic hydrocarbons (benzene, toluene and xylene isomers) to better assess their transfer in the environmental compartments (air, water, sediment and biota). A fugacity based calculation model was applied to establish the bio-concentration factors (BCFs) that relates the compounds concentration from sediment-, water- or air- to the biota based on experimental data. Thus, conclusive suggestions can be achieved for a rapid preliminary risk assessment as support tool for the preventive measures in the contaminated areas resulting from accidental chemical discharges or continuous pollution. For thus, water and sediment samples were collected and analyzed by gas chromatography for the selected compounds, the results being applied as input data for the model. The modeling revealed the tendency of the investigated compounds to transfer from water section to air. Simulated values obtained for section sediment as validation tool, are comparable and compatible with the values obtained by analytical measurements, and thus a rapid estimation of the pollution level in the environmental compartment of interest can be achieved based on a limited number of analytical measurements. Thus, by applying the fugacity model to estimate a pollution footprint, conclusive indications for a rapid environmental risk assessment can be achieved.*

**Keywords:** volatile organochlorine substances, volatile aromatic hydrocarbons (BTEXs), MacKay model, fugacity, ecosystem

Environmental pollution with hazardous substances occur mainly due to wastewater discharges from point sources and diffuse emission sources containing non-synthetic pollutants (heavy metals) and/or synthetic pollutants (organic micro-pollutants). Hazardous substances produce toxicity, persistence and bio-accumulation in the aquatic environment. Volatile organic compound are widely used in industry, given their evaporation ability after use. The large amounts of organochlorine substances are obtained during the chlorination of drinking water and wastewater. Although it was found that are over 200 natural halogenated hydrocarbons, most chlorinated compounds into the environment are of anthropogenic origin [1]. As these substances progresses in the food chain, their concentration increases the risks to human and ecosystem following the same trajectory. Therefore, the control of emissions of these substances, even when they are in very small amounts may become a necessity [2-4].

The level of contamination resulting from accidental or continuous chemical discharges was usually assessed using the 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 [5-8]. One such model is the MacKay model [9, 10], which uses patterned backgrounds to explore the possible behaviour of the chemical and thus may estimate the level of pollution

with hazardous chemicals to environmental water, sediment, and biota. This model can give conclusive hints for a rapid risk assessment on which to support conclusions on the pollution preventive measures. Effective management requires understanding of the environment and the ability to analyze quantitative risk transfer mechanism associated to health and chemical contamination.

Environmental models are important tools in understanding the behavior of contaminants in complex environments. They are used to simulate chemical transport with focus on a single medium and multimedia fate models, allowing to calculate the chemical behavior in various environmental compartments. The multimedia fate model (MFM), as originally developed by Mackay [11], is a general multimedia model that has been applied to various environmental systems [12] and has proven its usefulness in understanding the relations among different media. However, the general MFM is based on a box model that does not consider spatial variability. To combine the advantages of the single-medium model and the general MFM, previous studies have suggested watershed-based spatially resolved multimedia fate models based on an integration of a grid-based air advection model and a polygon shape watershed-based multimedia model.

The first level (Level I) of calculation evaluates the equilibrium distribution of fixed quantity of chemical between the compartments in a closed evaluative or *unit world* environment, i.e. equifugacity applies. It is a steady state calculation with no inflow, outflow, intermedia transport or degrading reactions. Output from the Level I

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calculation indicates the phases or media into which a chemical is likely to partition. It also provides equilibrium concentrations of the chemical in each compartment of the model environment and thus shows the media where concentrations are likely to be highest (i.e. the fugacity capacity,  $Z$ , is largest) and where the masses are highest (i.e.  $VZ$  is largest, where  $V$  is the compartment volume and  $Z$  is the corresponding  $Z$  value).

In 1983, a set of two papers was published describing simple models of chemical fate in lakes and rivers [13], namely the QWASI (Quantitative Water Air Sediment Interaction) models. The models were compiled using the fugacity concept and have been made freely available as software from the website of the Canadian Centre for Environmental Modelling and Chemistry (CEMC) and have been widely applied to specific environmental systems [14, 15]. Chemical inputs are by direct emissions, adventive inflows of water and suspended particles, and deposition from an atmospheric compartment with a defined concentration by wet and dry aerosol and gaseous deposition. Steady state mass balance equations are compiled separately for the water and sediment compartments with chemical masses and concentrations expressed as fugacities in water and in sediment. Although the model simulates a steady state condition it can be adapted to treat dynamic conditions as a pair of first order differential equations that can be solved analytically or numerically [16, 17].

In previous studies [16-18] we described an updated state of the science EQUilibrium Criterion (EQC) model that is used to provide a screening level evaluation of the likely fate of a chemical that is introduced into a multimedia environment by various modes of entry.

This work focuses on a *fugacity* based calculation model useful to assess the bio-concentration factors (BCFs) that relates the pollutant compounds concentration from sediment-, water- or air- to the biota based on experimental

data. The application was performed on the Olt River, in its middle and lower catchment, considering the volatile organic compounds (1,2-dichloroethane and perchloroethylene) and volatile aromatic hydrocarbons (benzene, toluene and xylene isomers) in water and sediments as input data to better assess their transfer in other environmental compartments, like air and biota.

## Experimental part

### Materials and methods

#### Study area and sample collection

The Olt River, the main tributary of the Danube River in Romania, has a total length of 615 km and from its source in the Eastern Carpathian Mountains (Harmas orographic node) to its flows in the Danube (at Islaz) passes relief units with various physical and geographical features (30% mountains, 53% hills and 17% plain). Our study refers to the middle and lower watershed of the Olt River, from Cornetu (North of Valcea county) to Islaz (South - the point of flowing in the Danube). There are 25 cascading dams constructed on the river for flood control, energetic and irrigation purposes, which can considerably affect the river flow. The climatic conditions of the study area are somehow influenced by the varied relief in the catchment of the Olt River and also the anthropogenic activities are diverse.

For this study water and sediment samples were collected in 22 points (Fig. 1), including 19 accumulation lakes, during the springtime of year 2018. The sampling was performed under snow (in March) and rain (in May) conditions also accentuated by the significant rise in temperatures, from an average of 6°C in March to 22°C in May 2018, which can influence the concentrations of the investigated compounds.

Water samples were collected in polyethylene bottles, at depth between 0.2 and 0.5 m while sediments were sampled into plastic bags, and preserved by adding a small amount of concentrated nitric acid.

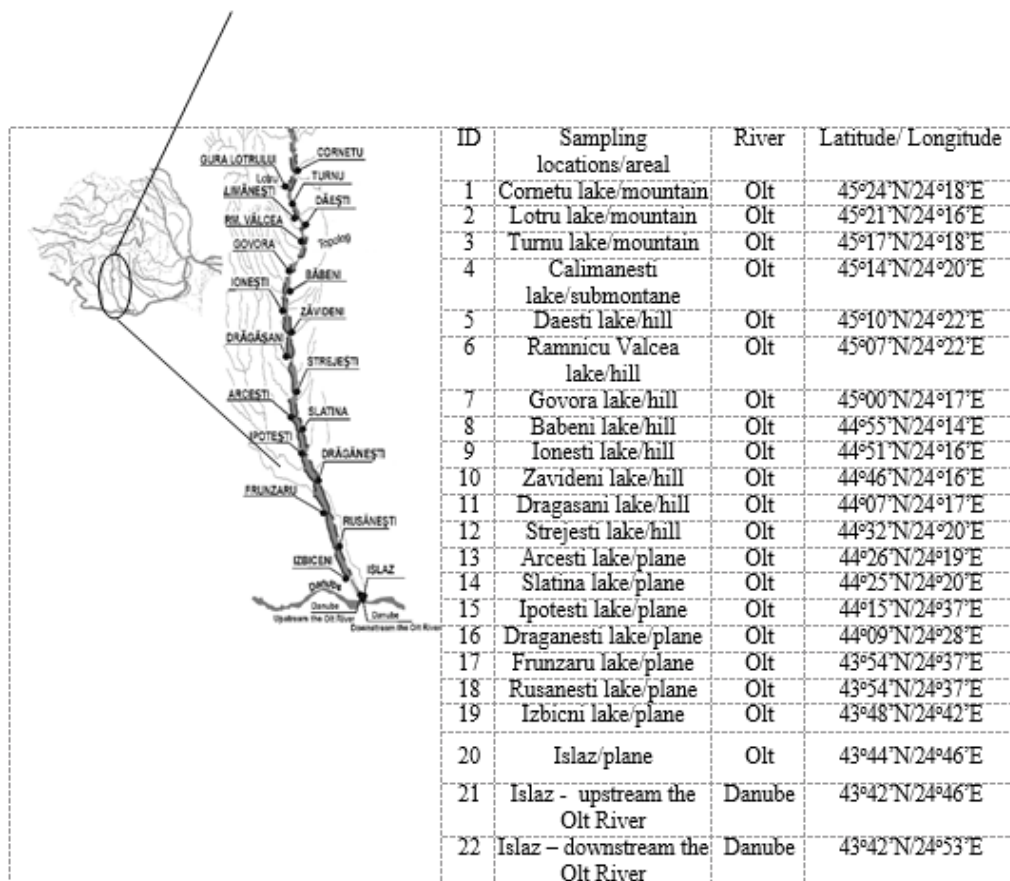


Fig. 1. Investigation area - localization of water and sediments sampling points

## Samples collection and chemical analysis

### Samples preparation

Concerning the VOCs sample preparation: we took in account 500 mL of water which was extracted twice with 50 mL of hexane. The combined extracts were dried over on sodium sulfate and concentrated to 2 mL with a TURBOVAP concentrator, and then introduced for analysis by GC/MS. For the BTEX water preparation we needed 10 mL of water which was extracted with 2 mL of hexane and the extract was dried over sodium sulfate and injected into GC/MS. For sediments no preparation procedure was applied. The samples were directly quantified by contribution of dynamic HEADSPACE GC/MS analysis.

### Analytical procedure

The analytical investigation of the chlorinated organic compounds and BTEX was performed using a Gas Chromatograph coupled with a Mass Spectrometer of 240-MS 450 GC Varian. For the chromatographic separation, a TG-WAXMS Polar Chromatographic Column with dimensions of 60 m x 0.32 mm x 0.25 μm was used.

For the analysis of chlorinated organic compounds (1,2-dichloroethane and perchlorethylene), the oven temperature was maintained at 70°C for 0.8 min, increased to 110°C at a rate of 3°/min, then 140°C at 3°/min and increased to 160°C by 1.2°/min where the duration was 2 min. In case of volatile aromatic hydrocarbons (benzene, toluene and xylene isomers), the oven temperature was maintained at 40°C for 1.2 min, increased to 90°C at a rate of 10°/min then 120°C at 5°/min and increased to 200°C by 10°/min where the time duration was 10 min.

### Model application

General data regarding the fugacity concept

The multimedia QWASI model was created by the Canadian Centre for Environmental Modelling and Chemistry and is used to calculate the changing trend of chemicals in the environment [19]. However, this method is only applicable for chemicals with a measurable vapor pressure. For most nonvolatile chemicals, such as heavy metals, an equivalence approach is used instead. Briefly, the model is based on mass conservation (the water body is well mixed), by means of defining a series of Z values (equivalence capacity, dimensionless) and D values (transfer parameters, m<sup>3</sup>/d), using Q (equivalence, mole/m<sup>3</sup>) as the equilibrium criterion, and creating the mass balance equation for the liquid (water), solid (sediment), and air phases under steady or unsteady states.

In order to study the distribution of chemicals in various environmental matrices also a qualitative description of the types of matrices is required, highlighting some of the most important physico-chemical properties. In this sense, averages *model* are put together and could be used later in the calculations. For calculus an area of 1km/1km is considered, including air, water, soils and sediments. These environments have assigned volumes and typical properties, purely illustrative and that, in turn necessitated some changes if was treated chemical evolution in a specific region [8, 9].

According to G.N. Lewis [20], the 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) [9]:

$$P_T V = nRT \quad (1)$$

where Z is a constant of proportionality called *fugacity capacity* with the units mol/m<sup>3</sup>Pa. 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* - The basic equation for the fugacity [9] of a substance in the state of the vapor is:

$$F = y \times \phi \times P_T \quad (2)$$

where y is the mole fraction of chemicals and fugacity coefficient φ is P<sub>T</sub> is the pressure (atmospheric) total.

Considering the law of gases:

$$P_T V = nRT \quad (3)$$

where n is the total number of moles of air and chemicals present, and T is the absolute temperature, the chemical concentration C (solute) will become:

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

Thus,

$$Z \text{ is } \frac{1}{\phi RT} \quad (5)$$

or

$$\frac{1}{RT} \quad (6)$$

when the Φ=1.

*Fugacity (Z) for water* - Fugacity equation for a compound i dissolved in water or another solvent is given in terms of mole fraction x<sub>i</sub>, activity coefficient γ<sub>i</sub> and reference fugacity f<sup>R</sup> based on Raoult law as (eq. 7-14):

$$f = x_i \gamma_i f^R \quad (7)$$

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

$$V_w = n_w v_w \quad (9)$$

$$x_i = \frac{n_i}{n_i + n_w} \approx \frac{n_i}{n_w} \quad (10)$$

where i - solute, and w - water

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

$$f = C_i v_w \gamma_i f^R \quad (12)$$

or,

$$C_i = \frac{1}{(v_w \gamma_i f^R) f_i} \quad (13)$$

$$Z_i = \frac{1}{v_w \gamma_i f^R} \quad (14)$$

For a solution in water Z<sub>w</sub> may be inferred as (eq. 15-17):

$$Z_w = \frac{1}{v_w \gamma_i P_{SL}} \quad (15)$$

$$K_{aw} = \frac{Z_A}{Z_w} = \frac{H}{RT} = \frac{P_s}{C_s RT} \quad (16)$$

$$Z_w = \frac{Z_A RT}{H} = \frac{1}{H} = \frac{C_s}{P_s} \quad (17)$$

(because  $Z_A = \frac{1}{RT}$ ),  $C_s$  and  $P_s$  situation where are values for liquids and solids status.

**Fugacity (Z) for the soil or sediment** - The simplest method of deduction for Z is correlating him for  $Z_{water}$  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):

$$C_s = K_{sw} C_w \quad (18)$$

where  $C_s$  is the concentration of adsorbed ( $\text{mol/m}^3$  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  $\rho_s$  in l/g/L (or  $\text{g/cm}^3$  or  $\text{mg/m}^3$ ) as follows:

$$K_{sw} = \rho_s K_p \quad (19)$$

$$K_{sw} = \frac{Z_s}{Z_w} \quad (20)$$

$$Z_s = Z_w K_{sw} = \frac{\rho_s K_p}{H} \quad (21)$$

**Fugacity (Z) for biotic phase (fish)**

$$Z_b = \frac{\rho_b K_{bw}}{H} \quad (22)$$

$\rho_b$  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 procedures for estimating the Z values is performed for each environmental situation

again, then the equilibrium concentrations can be derived using  $f$  as a common criterion of balance.

## Results and discussions

### Model parameters

Starting from measured values of the investigated pollutants in environmental compartment [22-26] *water* the transfer of these hazardous pollutants in *sediment*, *biota* and *air* was achieved by modeling. To validate the model, also the measured values obtained for *sediment* samples were used, as these types of evidence have been worked as real samples in the laboratory. Biota has an approximate quantity of 1 part/ $\text{m}^3 = 7.83 \times 1 \text{ million } 107/106 = 78.3$ . The input data to the model comprised environmental parameters describing the compartment composition, inter-compartment exchange rates, etc., physicochemical properties of volatile organic compounds (1,2-dichloroethane and perchlorethylene) and volatile aromatic hydrocarbons (benzene, toluene and xylene isomers) and emission data. The values of physicochemical properties of volatile organic compounds (1,2-dichloroethane and perchlorethylene) and volatile aromatic hydrocarbons (benzene, toluene and xylene isomers) used here were the mean values derived from previous studies [21] or most frequently used in the model calculation. The main physicochemical properties (vapor pressure ( $P_s$ ), n-Octanol/Water Partition Coefficient ( $K_{ow}$ ), water-soil partition coefficient ( $K_{oc}$ ), organic carbon partition coefficient ( $K_d$ ), water-soil partition coefficient ( $K_d$ ) and Henry's law ( $H$ ), of investigated compounds, used in the modeling are summarized in Tables 1 and 2.

### Transfer of COVs to the environment of Olt River

The mathematical model was applied to the organochlorine substances: 1,2 dichloroethane and perchlorethylene. The results of simulation are highlighted in Fig. 2, highlighted the tendency for the volatile organic compounds, 1,2-dichloroethane and tetrachloroethane, known to be volatile compounds, to accumulate in the *air* compartment, at values of 65% for 1,2-dichloroethane and 68% for perchlorethylene.

Starting from the measured values of these pollutants in the environmental factor *water*, by applying the fugacity model, the transfer of these hazardous pollutants in environments *sediment*, *biota* and *air* was achieved (Fig. 3). For model validation, the measured values of the pollutants in the sediment samples were used.

**Table 1**  
PHYSICOCHEMICAL PROPERTIES OF VOLATILE ORGANIC COMPOUNDS (1,2 -DICHLOROETHANE AND PERCHLORETHYLENE) [21]

Symbol	Unit	1,2 – dichloroethane	Perchlorethylene
$P_s$	Pa	8700	1900
$K_{ow}$	-	28.18	2511.88
$\text{Log } K_{ow}$	-	1.45	3.40
$K_{oc}$	-	38.02	95.50
$K_d$	-	0.1901	0.4775
$H$	$\text{Pa} \cdot \text{m}^3/\text{mol}$	98.96	1529.41

**Table 2**  
PHYSICOCHEMICAL PROPERTIES OF VOLATILE AROMATIC HYDROCARBONS (BENZENE, TOLUENE AND XYLENE ISOMERS) [21]

Symbol	Unit	Benzene	Toluene	Ethylbenzene	o-xylene	m-xylene	p-xylene
$P_s$	Pa	10000	3780	900.0	700.0	800.0	900.0
$K_{ow}$	-	125	562.34	1380.38	1318.25	1584.9	1412.5
$K_{oc}$	-	134.9	140.0	204.0	239.9	199.52	199.50
$K_d$	-	0.675	0.700	1.02	1.119	0.998	0.998
$H$	$\text{Pa} \cdot \text{m}^3/\text{mol}$	436.37	662.15	562.08	412.88	530.85	579.11

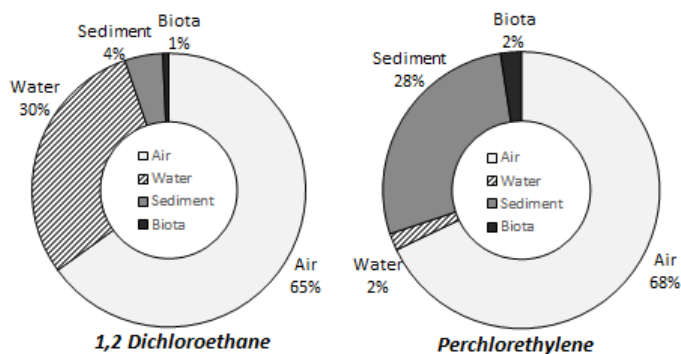


Fig. 2. Transfer of 1, 2 - dichloroethane and perchlorethylene in the environmental compartments (air, water, sediment, and biota)

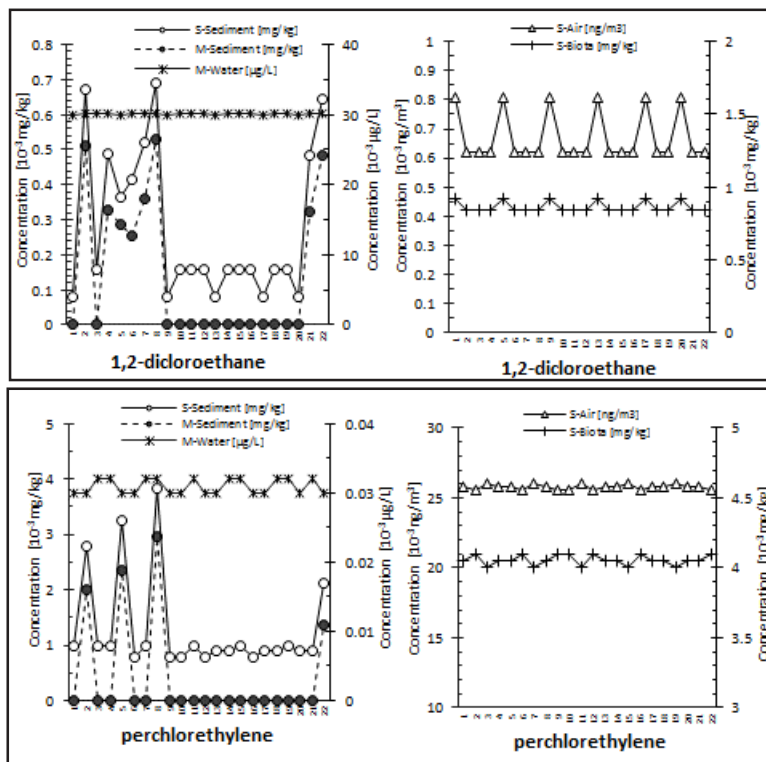


Fig. 3. Measured/predicted concentration of 1,2-dichloroethane and perchlorethylene in environmental compartments

**Transfer of 1,2-dichloroethane** - the values obtained for the environmental *sediment* in the modelling transfer of 1,2-dichloroethane from water was very similar to those determined experimentally in the measurement campaigns: e.g. 0.00016 mg/kg by simulation, <0.0001 mg/kg (the detection limit of the method) by measurement. As overall observation, the simulated values of 1,2-dichloroethane concentration in *sediment* (e.g. 0.00016 mg/kg) were slightly higher than those determined experimentally during the measurement campaign, of <0.0001 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 <0.0001 mg/kg. From the modelled values was observed a tendency by transfer of 1,2-dichloroethane in the section *air*, with values between 0.030-0.03017 ng/m<sup>3</sup>; insignificant amount is taken from the *biota* compartment, with values between 0.001 to 0.00084 mg/kg.

**Transfer of Perchlorethylene** - the values obtained for the environmental *sediment* in the modelling transfer of perchlorethylene in water are close to those determined experimentally (e.g. between 0.001 mg/kg and 0.00078 mg/kg by simulation to <0.001 mg/kg and 0.0036 by measurement). The values obtained from measurements were slightly lower than the simulated ones for the transfer of perchlorethylene from water to *sediment*. From the modelled values was observed a tendency by transfer of this pollutant in the section *air*, with values between 0.02561 to 0.0026 ng/m<sup>3</sup>;

insignificant amount is taken from the *biota* compartment, with average value of 0.004055 mg/kg.

#### *The transfer of BTEXs compounds in the environment of Olt river*

The mathematical model was developed for analysis of benzene (B), toluene (T), ethylbenzene (E), and isomeric (*o*-, *m*-, *p*-) xylenes (X). The values of the modelling are presented in figure 4. Was observed that the volatile aromatic hydrocarbons (BTEXs) have a transfer tendency in the air of 84.3% for benzene, 77% for toluene, 58% for m-xylene, 57% for ethylbenzene, 53% for m-xylene and 51% for o-xylene.

Starting from the measured values of these pollutants in environmental factor *water* was achieved by modelling their transfer to the environmental compartments *sediment*, *biota* and *air*. Of course, to validate the model, real values obtained by measurements for *sediment*, were considered. The obtained results are presented for each sampling point in figure 5-10.

For benzene (Fig. 5), the values obtained by modelling for *sediment* (average 0.0000678 mg/kg) were in agreement with those obtained by measurement, except for 5 sampling points, namely Calimanesti, Daesti, Ramnicu Valcea, Govora and Babeni, where higher values were registered, of 0.0163 mg/kg, 0.0255 mg/kg, 0.0157 mg/kg, 0.0255 mg/kg and 0.0157 mg/kg respectively. From the modelled values was observed a tendency by transfer of benzene in the section *air*, with values between 0.002 to 0.026 ng/m<sup>3</sup>; insignificant amount is taken

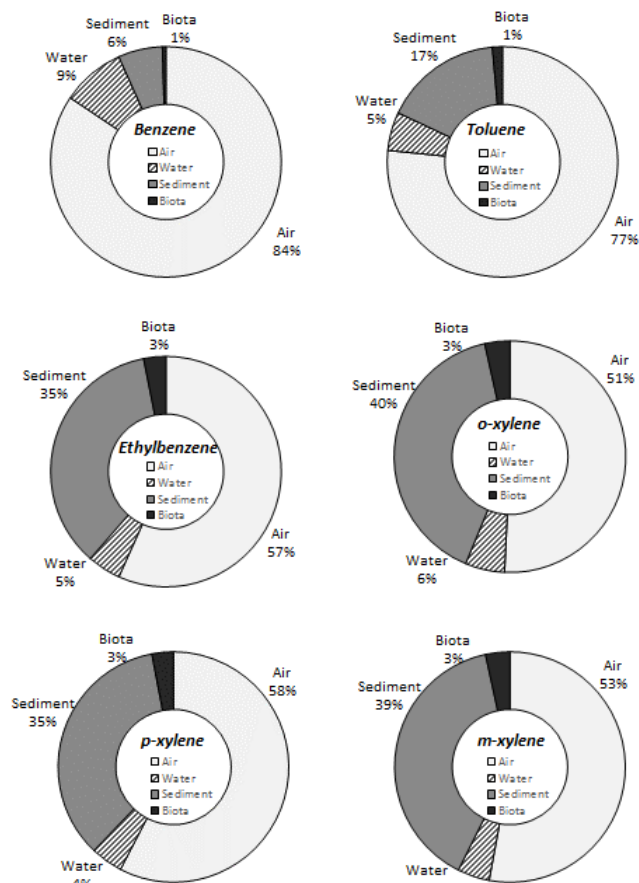


Fig. 4. The transfer of BTEX in the environmental compartments (air, water, sediment, and biota) of the Olt River (middle and lower basin) areal

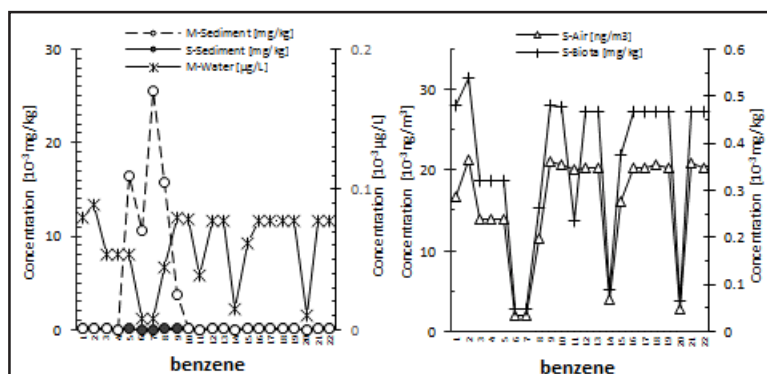


Fig. 5. Measured/predicted concentration of benzene in environmental compartments

from the *biota* compartment, with average value of 0.000353 mg/kg.

By simulation, the results for ethylbenzene (Fig. 6) in sediment (average 0.001392 mg/kg) were in agreement with those obtained by measurement ( $<0.005$  mg/kg), except for 6 sampling points, namely Calimanesti, Daesti, Ramnicu Valcea, Govora and Ionesti, where higher values were obtained, of 0.0267 mg/kg, 0.0157 mg/kg, 0.0208 mg/kg, 0.0197 mg/kg and 0.0201 mg/kg respectively. From the modelled values was observed a tendency by transfer of ethylbenzene in the section *air*, with values between 0.02158 to 0.03762 ng/m<sup>3</sup>; low amounts is taken from the *biota* compartment, with average value of 0.007278 mg/kg.

For m-xylene (Fig. 7), the values obtained by modelling for sediment (average 0.0014 mg/kg) were in agreement with those obtained by measurement ( $<0.003$ ), except for 4 sampling points, namely Govora, Dragasani, Izbiceni and Ipotesti where 0.137 mg/kg were registered. From the simulation was observed a tendency by transfer of m-xylene in the section *air*, with an average value of 0.025412 ng/m<sup>3</sup>; low amount is taken from the *biota* compartment, with average value of 0.007406 mg/kg.

The results achieved for o-xylene (Fig. 8) in sediment (average 0.001273 mg/kg) were in high agreement with the ones obtained by measurement ( $<0.003$ , the quantification limit of the method), except for Babeni sampling point where a value of 0.0069 mg/kg was obtained. The simulation also showed the tendency transfer of o-xylene in the section *air*, with an average value of 0.0001 ng/m<sup>3</sup>; low amount is taken from the *biota* compartment, with average value of 0.006791 mg/kg.

For p-xylene (Fig. 9), the values obtained by modelling for sediment (average 0.001326 mg/kg) were in agreement with those obtained by measurement ( $<0.003$  mg/kg), except for 4 sampling points, namely Ramnicu Valcea, Babeni, Zavideni, Danube – downstream the Olt River after flowing in the Danube River where higher values were registered, of 0.0102 mg/kg and 0.0187 mg/kg. From the modelled values was observed a tendency by transfer of p-xylene in the section *air*, with values below 0.0001 ng/m<sup>3</sup>; low amount is taken from the *biota* compartment, with average value of 0.006977 mg/kg.

In case of toluene (Fig. 10), the values obtained by simulation for sediment (average 0.000946 mg/kg) were in almost agreement with those obtained by measurement

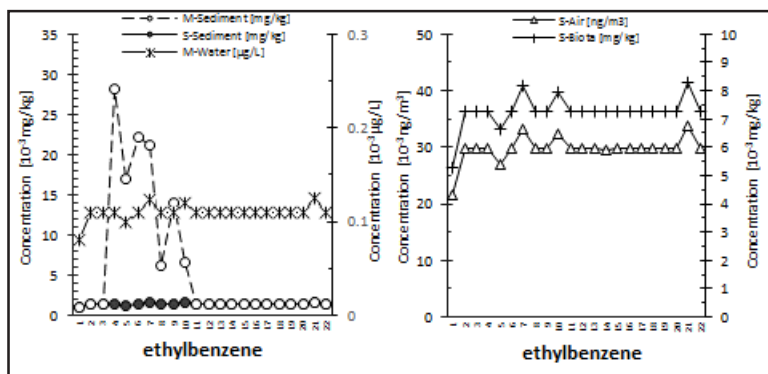


Fig. 6. Measured/predicted concentration of ethylbenzene in environmental compartments

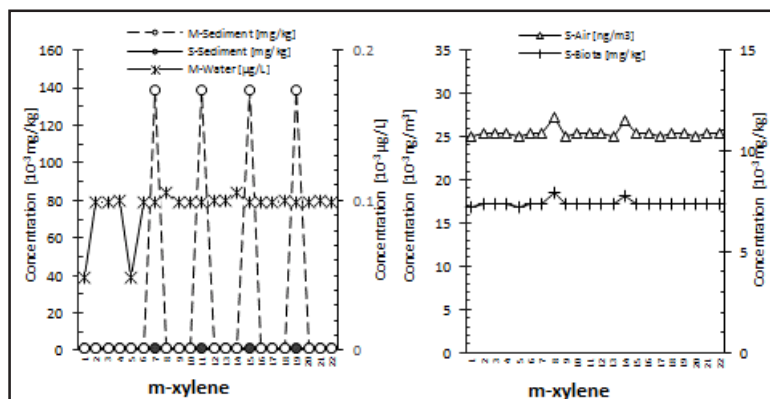


Fig. 7. Measured/predicted concentration of m-xylene in environmental compartments

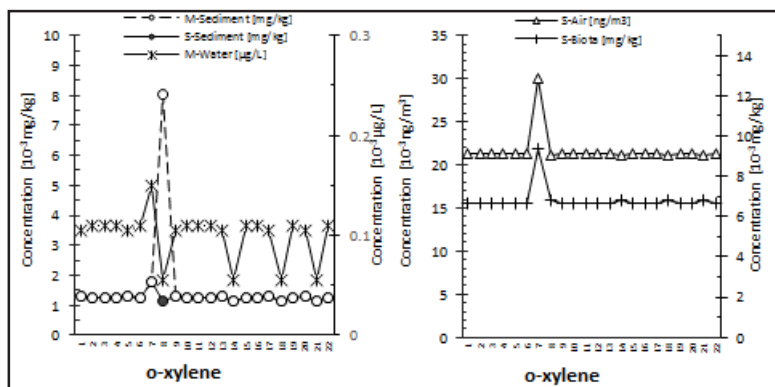


Fig. 8. Measured/predicted concentration of o-xylene in environmental compartments

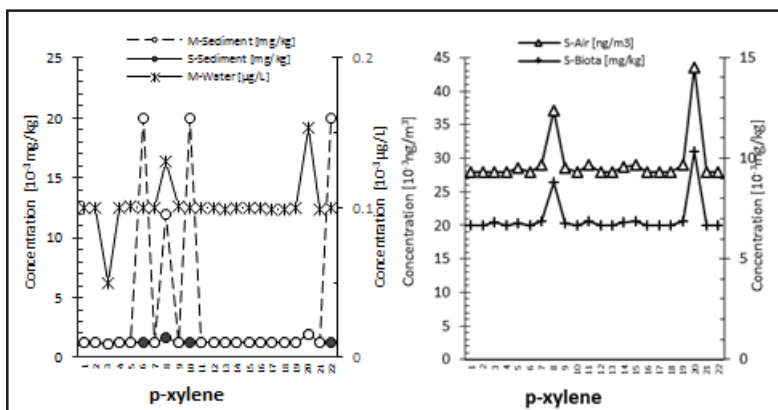


Fig. 9. Measured/predicted concentration of p-xylene in environmental compartments

(<0.003 mg/kg), except for Calimanesti (0.1491 mg/kg), Daesti (0.0121 mg/kg), Ramnicu Valcea (0.0147 mg/kg), Govora (0.0204 mg/kg), Ionesti (0.0121 mg/kg), Frunzaru (0.0102 mg/kg), Strejesti (0.0177 mg/kg), Islaz (0.0385 mg/kg), Danube -upstream the Olt River before flowing in the Danube River (0.079 mg/kg), and Danube -downstream the

Olt River after flowing in the Danube River (0.0227 mg/kg) where higher values were registered, of 0.0102 mg/kg and 0.0187 mg/kg. From the modelled values was observed a tendency by transfer of toluene in the section air; with values below 0.000197 ng/m<sup>3</sup>; low amount is taken from the „biota” compartment, with average value of 0.003879 mg/kg.

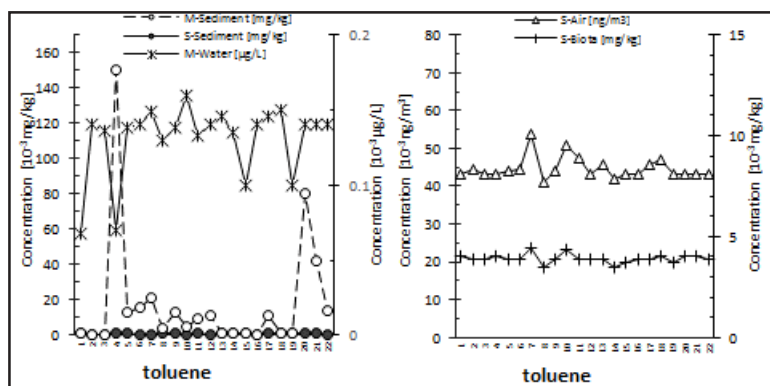


Fig. 10. Measured/predicted concentration of *toluene* in environmental compartments

## Conclusions

The applied model based on *fugacity* generated realistic indicative values for transfer of pollutants in environmental compartments of interest, respectively, air, sediment, and biota. The modelling values obtained for the *sediment* compartment are comparable and compatible with the values obtained through analytical measurements, which gives a quick indication of the pollution level with the precise pollutant in the studied compartment;

The modelling highlighted the trend of transfer in the *air* compartment of COV and BTEX in the sediment compartment. It highlighted the tendency of transfer of the volatile organic compounds, 1,2-dichloroethane and perchlorethylene (65.0% and 68% respectively), known to be volatile compounds, in the *air* compartment.

For the volatile aromatic hydrocarbons (BTEXs), a transfer tendency in the air of 84.3% benzene, 77% toluene, 58% m-xylene, 57% ethylbenzene, 53% m-xylene and 51% o-xylene was achieved.

For the validation of the modelling, the values obtained for the sediment factor were considered, as these types of samples could be analyzed as real samples in the laboratory. The simulated and measured data were in agreement with except of few cases, when measured values were lower than the estimated ones.

For a quickest and easiest applicability, the applied model did not make detailed calculations to include river flow, so the dilution factor can vary from one monitoring campaign to another, depending on the annual meteorological factors.

Using this type of modelling, that imply reduce number of analytical measurements, a fingerprint of environmental pollution can be estimated, supplying thus conclusive indications for a rapid risk assessment and a base for actions and preventive measures.

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