EVALUATING THE FATE OF PCBs IN THE SOUTHEAST REGIONAL PARK OF MADRID, SPAIN.

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1. INTRODUCTION.

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For a long time, many chemicals have been entered in the environment due to the beneficial aspects that their use provide to the agriculture, the industry, etc., but at the same time it has been evident that many of them, clearly, damage the environment and their effects persist for many years after exposure. A well known example of such chemicals are the PCBs. These compounds have been widely used since 1929 as dielectrics in electrical components, in hydraulic and vacuum pump fluids and as various additives, diluents and flame retardants (1). Their use was banned or limited (to closed systems) when it was discovered their persistence and their accumulation in animal fatty tissues, more important as we are higher in the trophic chain.

Mathematical modelling and simulation have been offered as tools for the prediction of chemicals fate as an integral part of their risk analysis, and in this way, Mackay's fugacity models (2,3) produce estimates where the contaminants will end up and whether accumulation in a component may be significant or not (3). These models employ the fugacity concept, that is, the escaping tendency of the chemical from a phase and consider the world as divided in compartments.

In this work, our aim is the evaluation of the fate of some PCBs congeners (101, 138, 153, 170 and 180) in the southeast regional park, Madrid (Spain) by means of a Mackay's fugacity model (level III), and its validation by comparing the predicted concentrations values with the experimental ones, measured in water, soils and sediments.

2. METHODS.

2.1. Description of model compartments.

The place under study is a zone inside a regional park protected by the Spanish Government near Madrid (Figure 1).

Four compartments have been considered, that is, air, water, soil, and sediments. Also, in the air phase a subcompartment, aerosol, has been considered. The water consists in water from the river, water from the aquifer, suspended sediments and fish. Soils contain solids, air and water and sediments are divided in solids and water.

All compartments are assumed to be well mixed and thus have a constant spatial concentration.



Figure 1. The southeast regional park of Madrid.

2.2. Model inputs.

In addition of the zone characteristics the model needs some physicochemical parameters for the chemicals and different transport velocities between phases. These parameters have been taken from the literature (4-6).

We have considered that the emission of PCBs takes place only from the river, neglecting air, soil and sediment emissions. So, the emission value has been determined from the experimental concentration value in the first sample point of the place under study (see Figure 1).

2.3 Model calculations.

The PCBs predicted concentrations have been calculated by means of a program in Excel (7).

In order to validate the model, the results have been compared with the experimental ones (available for water, soils and sediments, ref. (8)).

Also, the sensitivity analysis for the model has been achieved (9). It consists in varying some parameter values in order to know, what of them, influences in a major way the predicted concentration values. So, this information is valuable to know those parameters that should be measured or estimated with better precision.

3. RESULTS AND DISCUSSION.

The results obtained for PCBs 101, 138, 153, 170, and 180 are shown in Table 1. In this table, the experimental concentration values are also shown. A good agreement between calculated and experimental concentrations for water and sediments can be observed while a great difference between these values for soils can be viewed. This difference can be due to several facts, i.e., the concentration data were determined in a year in which the rain was unusually frequent, so some parameters used in the model, as soil-water run-off or soil-solids run-off can be inadequately low.

490

· · · · · · · · · · · · · · · · · · ·	РСВ	Air Conc. g/m ³	Water Conc. ng/ml	Soil Conc. ng/g	Sediment Conc. ng/g
101	Calculated	1.89 10 ⁻⁶	1.15	31.85	21.3
	Experimental range	nd	1.17-3.27	0.111-0.204	10.84-31.60
138	Calculated	7.72 10-7	0.438	24.34	21.1
	Experimental range	nd	0.5-1.29	0.012-0.151	1.59-16.15
153	Calculated	1. 7 9 10 ⁻⁷	0.287	13.19	16.1
	Experimental range	nd	0.49-1.02	0.089-0.154	3.60-6.29
170	Calculated	1.04 10-7	0.106	5.35	9.1
	Experimental range	nd	0.01-0.31	0.009-0.021	0.24-4.25
	Calculated	3.26 10 ⁻⁷	0.359	20.65	32.3
180	Experimental range	nd	0.36-1.34	0.045-0.091	0.74-5.37

 Table 1. Calculated and experimental concentrations in air, water, soil, and sediments.

nd: no determined

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Moreover, the soil volume has been calculated considering a depth of 1.5 m of the soil, that is the maximum depth of the sampling study. Although a premise of the model is the spatial unvariability of concentrations, our experimental data indicate that the highest contamination is located at a few centimeters from the top of the soil. But even at 1.5 m from the top PCBs concentrations differ from zero values. So, it is possible to think that the particular hidrology of the zone, with very porous soils, makes possible that contaminants migrate even deeper.

PCB concentrations in soil also depends, strongly, on the half life in the soil. Mackay et al. (4) indicates that the half-life of a chemical in the environment depends not only on the intrinsic properties of the chemical, but also on the nature of the surrounding environment. Factors such as sunlight intensity, hydroxyl radical concentration and the nature of the microbial community, as well as temperature, affect the chemical's half-life so it is impossible (and misleading) to document a single reliable half-life (4).

In this way, we can show, as an example, the results of the sensitivity studies of PCB 170 when its half-life in the soil is considered (Figure 2). It can be observed that as the half-life in the soil enhances the concentration of the chemical in air, water, and sediments does not vary, but the soil concentration enhances in an important way. This fact has also been observed for the

other chemicals, although the results have been not shown.

Some other variables affects the chemical concentration in the different compartments. As



half-life

an example, the following can be cited: the temperature, the melting point and the solubility in the soil PCBs concentration, the octanol-water partition coefficient and the half-life of PCBs (in the sediment) on the sediment compartment, etc.

Among the different transport velocities considered in the sensitivity studies, those that affect in a most important way are airside-air water MTC, water side-air water MTC, aerosol deposition and sediment deposition, so these values should be known precisely.

Our results indicate that the contaminants clearly accumulate in soil and sediments due to their affinity for the organic material in those phases.

Figure 2. Concentration of PCB 170 in the different Moreover, the fugacity model used in compartments as a function of its half-life in the soil. this study predicts concentration of the contaminants in the different phases considered very closed to the experimental ones, although more work is needed with respect to that in the soil.

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ORGANOHALOGEN COMPOUNDS Vol. 36 (1998)

492