Pesticide sorption and the transport processes in soils, connecting by buffer capacity

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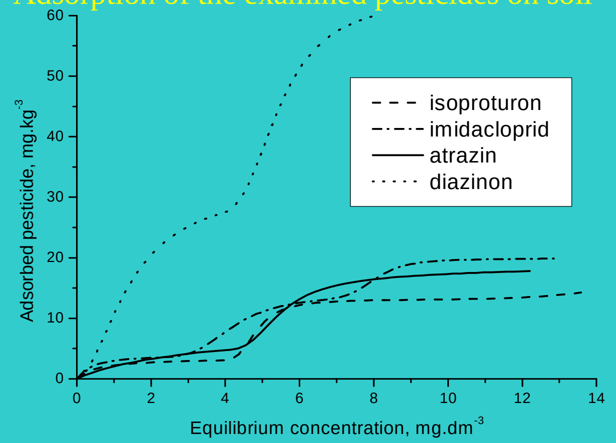
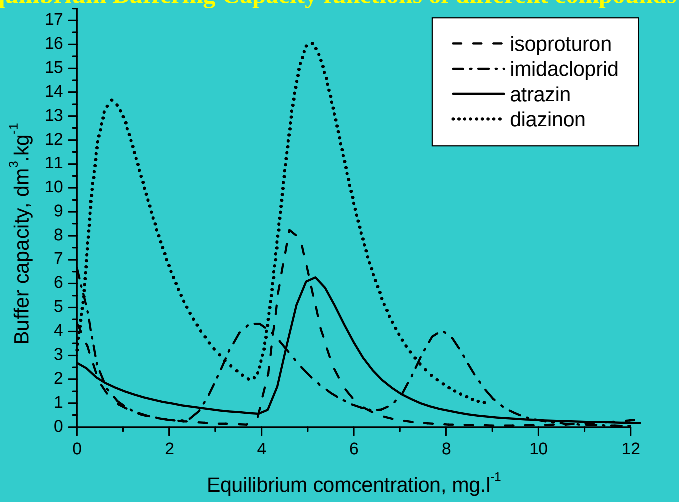
Using measured adsorption data we could calculate multi-step adsorption isotherms for different pesticides. Using and interpreting the multi-step isotherms, we derived formulas to calculate the Equilibrium Buffering Capacity of soil. These buffer capacity equations show interesting curves with one or more peaks. We could recalculating the measured and fitted values using real soil parameters. Based on these results we must redefine our original contamination assessment methods to avoid even a magnitude error. In addition to the equilibrium solution concentration measurement we need to know the Equilibrium Buffering Capacity (B) function as well for assessing the real amount of contaminants.

Adsorption of the examined pesticides on soil



Equilibrium Buffering Capacity functions of different compounds



When adsorbing isoproturon on the surface of the soil we get a three-step adsorption isotherm. In this case we can write generally the equation to describe the adsorption:

$$q=\frac{[a_1\cdot k_1\cdot c]^{n_1}}{[1+k_1\cdot c]^{n_2}}+\frac{a_2\cdot k_2\cdot[(c-b_2)+abs(c-b_2)]^{n_2}}{2^{n_2}+k_2\cdot[(c-b_2)+abs(c-b_2)]^{n_2}}+\frac{a_3\cdot k_3\cdot[(c-b_3)+abs(c-b_3)]^{n_3}}{2^{n_3}+k_3\cdot[(c-b_3)+abs(c-b_3)]^{n_3}}$$

The following equation describes the buffering capcity:

$$B=\frac{a_1\cdot k_1\cdot n_1\cdot c^{n_1-1}}{\left\{1+k_1\cdot[c]^{n_1}\right\}^2}+\frac{2^{n_2}\cdot a_2\cdot k_2\cdot n_2\cdot[(c-b_2)+abs(c-b_2)]^{n_2-1}}{\left\{2^{n_2}+k_2\cdot[(c-b_2)+abs(c-b_2)]^{n_2}\right\}^2}+\frac{2^{n_3}\cdot a_3\cdot k_3\cdot n_3\cdot[(c-b_3)+abs(c-b_3)]^{n_3-1}}{\left\{2^{n_3}+k_3\cdot[(c-b_3)+abs(c-b_3)]^{n_3}\right\}^2}$$

To calculate the changing the amount of pollution of a compound in solid phase in a given water content of soil, we use:

$$dQ=\frac{1-\Theta}{\Theta}\cdot EBC\cdot dc$$

where

- dq is the change of the pollution amount in solid phase, $mg.kg^{-1}$
- dc is the change of the concentration of solution, $mg.dm^{-3}$
- EBC is the Equilibrium Buffering Capacity, $dm^3.kg^{-1}$
- Θ is the water content of soil, $dm^3.dm^{-3}$

To calculate the total adsorbed amount (in milligrams) of the compound in the soil, we must add the solid phase and liquid phase content.

$$dQ=\frac{1-\Theta}{\Theta}\cdot V_{soil}\cdot\rho_{soil}\cdot EBC\cdot dc+\frac{\Theta}{1-\Theta}\cdot V_{soil}\cdot dc$$

Assuming that the soil water content is 0.2 - based on the isoproturon curve - if the equilibrium solution concentration increases from 2 mg.dm-3 to 2,1 mg.dm-3, the EBC is 0.35 dm3.kg-1. The change of total isoproturon content is **0.1 kg.** Under the same water condition and with the isoproturon buffer function, if the equilibrium solution concentration increases from 4.5 mg.dm-3 to 4.6 mg.dm-3, the EBC is 8.18 dm3.kg-1. The change of total isoproturon content is **21 kg.**

From an opposite point of view: let us assume that 20 kg.ha-1 isoproturon is added to the soil, presumably as a plant protection activity. If the original equilibrium solution concentration was 2 mg.dm-3 it is increasing by 2 mg.dm-3, i.e. **100 % increasing**, however if the original equilibrium solution concentration was 4,5 mg.dm-3 it is increasing by 0,1 mg.dm-3, i.e. **2 % increasing**.

The explanation of Equilibrium Buffering Capacity function of isoproturon