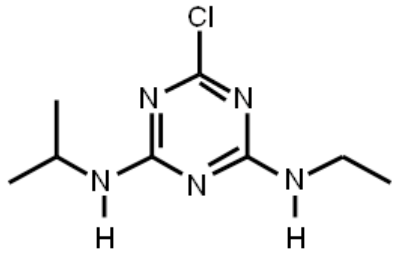
What fraction of atrazine is present in dissolved form?

Atrazine is still one of the most widely used herbicides worldwide. Estimate the fraction of total atrazine present in truly dissolved form (a) in lake water exhibiting 2 mg particulate organic carbon (POC) suspended per L water, (b) in marsh water containing 100 mg solids L^{-1}, if the solid's organic carbon content is 20%, and (c) in an aquifer exhibiting a porosity of 0.2 by volume, a density of the minerals of 2.5 kg L^{-1}, and an organic carbon content of 0.5%. Assume that partitioning to organic matter is the major sorption mechanism.

Use the following sorption constant for atrazine

$$K_{ioc} \cong 100 \ L \cdot kg_{oc}^{-1}$$



atrazine

If you are confused because you do not understand what to do with the organic carbon content and how to deal with phases that are not quantified by volume then it is high time to read chapter 3 in the textbook.

Question: What practical relevance do the results have?

Help: You can use spreadsheet C for all calculations: The total volume that you choose does not matter for the results. For simplicity take 1 litre and choose all other volumes according to the information given in the question.

If you want to do the calculation by hand use ...

- Excercises for an improved intuitive understanding
- Questions for recapitulation
- Good to know
- Minesweeper-problems

for (a) and (b): $$f_{iw} = \frac{1}{1 + S \cdot f_{oc} \cdot K_{ioc}}$$

S f_{oc} = [POC] (particular organic carbon),

S = particle concentration [kg S L^{-1}]

for (c): $$f_{iw} = \frac{1}{1 + \rho s \cdot \frac{1-\Theta}{\Theta} \cdot f_{oc} \cdot K_{ioc}}$$

Answer:

$$f_{iw} = \frac{1}{1 + 2 \cdot 10^{-6} \cdot 10^{2}} = 0.9998$$

(a) Practically all the atrazine is residing in the water phase. Relevance: 1) Sedimentation of POC in the lake will not be an effective transport mechanism for atrazine into the sediment and will not change the water concentration. 2) If you analyse a water sample it does not matter whether you extract the whole sample (including POC) or a filtered sample.

b) $$f_{iw} = \frac{1}{1 + 2 \cdot 10^{-5} \cdot 10^{2}} = 0.998$$

Although sorption is somewhat higher than in case a) it is still negligible. The conclusions from case a) still hold for marsh water.

c) $$f_{iw} = \frac{1}{1 + 10 \cdot f_{oc} \cdot K_{ioc}} = \frac{1}{1 + 10 \cdot (0.005) \cdot 10^{2}} = 0.17$$

In the aquifer, most of the atrazine is sorbed to the solid matrix of the soil. Hence, transport through the aquifer with the water is considerably slowed down (see Box 13 in the textbook).