

Quantitative equilibrium calculations

- Fundamentals
- Problems
- Excercises for an improved intuitive understanding
- Questions for recapitulation
- Good to know
- Minesweeper-problems
 - Question 1
 - Question 2
 - Help 1
 - Help 2
 - Question 3
 - Answer

Question 2

Most questions and exercises that you encounter here are given in a context and formulated in a way that already points you towards the correct answer. Real life is different. So every now and then we will also ask you a question (like the one that follows) that is closer to real-life situations. Take this challenge serious and spend some time thinking about the question before you use the help that we may also offer.

Can you say something about the amount of dust/soil that should be sampled in a REST procedure (see Chapter 2 for explanation) for each sample? Note, that it is not clear yet whether the dogs use DNT or TNT as signature compounds (In fact, there might be even other odours of importance but this goes beyond what we can cover here). The partition constants of TNT are also given below. There is some uncertainty in the $K_{\text{surface air}}$ -values of both, DNT and TNT. The real values might be higher by a factor 10. Consider this in your answer.

Use the following partition constants:

for DNT at 15°C:

- $K_{\text{wa}} = 1.39 \text{ E5 } [L_{\text{air}}/L_{\text{water}}]$
- $K_{\text{oc air}} = 6.7 \text{ E7 } [L_{\text{air}}/\text{kg}_{\text{oc}}]$
- $K_{\text{surface air}} = 1.3 \text{ E-2 } [m^3_{\text{air}}/m^2_{\text{surface}}]$
for mineral surfaces at 90% rH

and for TNT at 15°C:

- $K_{\text{wa}} = 6.0 \text{ E6 } [L_{\text{air}}/L_{\text{water}}]$
- $K_{\text{oc air}} = 1.4 \text{ E5 } [L_{\text{air}}/\text{kg}_{\text{oc}}]$
- $K_{\text{surface air}} = 1.3 \text{ E-1 } [m^3_{\text{air}}/m^2_{\text{surface}}]$
for mineral surfaces at 90% rH

Note, that the air/water partition constant is asked for in the spread sheet while the water/air partition constant has been given to you above.

Help 1: The previous question already points out the considerations that are important here. Ideally you will use so much dust that equilibration with the air during presentation will not lower the concentration in the soil substantially, because then also the equilibrium air concentration will be the highest you can reach. The answer depends on the air/soil partition constant of the considered compound and the volume of air that gets into equilibrium with the soil sample. As long as this volume of air is not known (it depends on the experimental set-up and would have to be measured) you can only say how much dust is needed per litre of air that has to be equilibrated.

Help 2: You might answer right away: The more soil the better. That is correct. However, when you do the quantitative calculations you will find that above a certain amount of soil, x, you may increase the amount of soil by a factor 10 with only a very tiny increase in the equilibrium air concentration. In this case using more soil would of course not be

desirable for many practical reasons. Hence, it is indeed possible to report an optimal amount of soil. (see also Box 3 in the script and [Excercises for an improved intuitive understanding](#))

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