## Quantitative equilibrium calculations

- Fundamentals
- Problems
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- 5 ml water instead of 1 ml
- 2 ml air volume instead of 1 ml
- 25 ml air volume instead of 5 ml
- ↓ 🛛 🧿 Volumes are doubled
- Total amount of the substance is doubled
- ↓ Initial situation changes
- Questions for recapitulation
- Good to know
- Minesweeper-problems

## Excercises for an improved intuitive understanding

After working through these problems you should have developed a good overview of how partition constants can be applied to solve quantitative partition problems. But do you also have a good 'intuitive' understanding of how partition systems respond to changes of one or several variables? If you change the volume of a phase or a partition constant then some of the system responses (like changes in equilibrium concentrations, mass fractions) are proportional to the changed variable while others are not. An example for a non-linear response is the fact that you will need 10 times more solvent to extract 99% of a chemical out of a water sample than if you wanted to extract only 90% (see problem <u>Organic pollutants in water</u>). The following exercise is intended to train your intuitive understanding of partition processes (corresponds to Box 3 in the script).

## Exercise for a better understanding of the system response of a simple partition system:

Use sheet 1 of the <u>Mehr-Phasensystem.xls</u> to calculate the equilibrium state of 1 ng of a compound *i* in the following partition system: 1 ml air, 1 ml water and a  $K_{i aw}$  of 0.1 [ $L_{water} / L_{air}$ ]. Try to estimate (not calculate yet) how the concentrations of *i* and the mass fraction of *i* in both phases change if you change the system as follows:

## What will happen if both volumes are doubled?

**Answer:** The distribution of the compound's mass stays the same but the concentrations are reduced to half of the original values.

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