Quantitative equilibrium calculations

- Fundamentals
- Problems

Excercises for improved understanding

- 5 ml water instead of 1 ml
- ↓ 0 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 Organic pollutants in water). 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 Mehr-Phasensystem.xls 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 $K_{i \text{ aw}}$ 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:

25 ml air volume instead of 5 ml

Answer: In this case the only safe conclusion is that the mass distribution will shift substantially towards the air phase and all concentrations will decrease.





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