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 $K_{i\,aw}$ 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:

5 ml water instead of 1 ml

Answer: The mass distribution of *i* must shift further to the water phase. It won´t change much though, because it had been dominated by the water phase already. In the new equilibrium the mass fraction in water must be between 91 and 100%. From that, one can conclude that the concentration in water must drop to about 1/5 of the original value because the mass of *i* in the water phase increases only little but the water volume is increased by the factor 5. If the water concentration drops to about 1/5 of the original value then the same must happen to the air concentration because otherwise the partition coefficient would not be valid any more. This in turn implies that the mass of *i* in the air also drops by a factor 5 because the air volume did not change. This eventually leads to the conclusion that the mass of *i* in water will be about 98%. Compare this with the exact solution of the problem (calculated with the spread sheet).