Quantitative prediction of K values

- Introduction
- Fragment models
- sp-LFERs
- pp-LFERs
- Comparison of the various methods
- Predictive models based on molecular structure

• Critical remarks on approaches from chemical engineeringh

- Selftest
- Problems
- ↓ Problem 1
- ↓ Problem 2
- ↓ Problem 3
- ↓ Answer
- ↓ Problem 4
- ↓ Answer
- ↓ Problem 5
- ↓ Answer
- ↓ Problem 6
- ↓ Answer
- ↓ Problem 7
- ↓ Problem 8
- ↓ Problem 9

Problem 5

Aerosols are a complex mixture of minerals, salts, water, organic matter and soot. Depending on the actual situation, sorption of organic pollutants from air to aerosols may be dominated by adsorption or absorption to one or several of these phases. You have collected 3 aerosol samples at various locations and measured sorption constants of nonane and decane at 25 °C. The results of $K_{jaerosol/air}$ in $[L_{air}/g_{aerosol}]$ are shown in the following table:

| | Sample A | Sample B | Sample C |
|--------|----------|----------|----------|
| nonane | 15 | 30 | 15 |
| decane | 48 | 96 | 70 |

What can you conclude from these results with respect to the properties of the aerosols?

Answer:

Only conclusions towards vdW interactions and (if applicable) the cavity energy (and thus the cohesive energy of the sorbent phase) are possible, because the alkanes are only sensitive to these two types of interaction. If sample B had different vdW interaction properties and/or cohesive energy then this would **not** effect both compounds proportionally. This is a general message that comes from the structure of the LSER equation. Every change in the sorbent properties will change the log K values proportionally which has an exponential effect on the K values. Thus we may conclude that sample A and B appear to be chemically similar with respect to vdW and cohesive energy of their sorbing components and only the absolute mass of their sorbing components is different. For example, sample A may contain 5% organic material and 95% salts, minerals and water which do not contribute significantly to the measured sorption while sample B contains 10% organic material (of the same type as sample A) and 90% salts, minerals and water which do not contribute significantly to the measured sorption. (Note, though that also dissimilar phases may have similar vdW and cohesive energies). In Sample C the sorbing phase must clearly be different from sample A and B because both compounds are not sorbing proportional to samples A and B.

