Equilibrium partitioning of organic compounds

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Question 2

2 a) In the text it was argued that the partitioning of chemicals that occur as pure phases (e.g. water) is not principally different from the partitioning of chemicals (most pollutants) that only occur at dilute concentrations within other existing phases. But why then is the partitioning of water into the air described by its saturation vapor pressure and not by a partition constant K water air/water (in [mol

 $^{/L}_{air}$]) or, as another example, why is the partitioning of water from its own phase into octanol described by its solubility in octanol (in [mol $_{water}$ /L $_{octanol}$]) instead of a partition constant K $_{water}$ octanol/water [L $_{water}$ /L $_{octanol}$]?

Answer: The partitioning of a chemical that occurs as a phase itself and not as a dilute solute in other phases is indeed a special case: Water in contact with a gas phase will evaporate until it reaches its equilibrium concentration in the gas phase. This equilibrium concentration depends on temperature and the interaction energy between the water molecules in their own phase. So far this is completely analogue to the partitioning of a dilute chemical. However, unlike a dilute compound that partitions from one phase into another the **Concentration** of water in its liquid phase stays the same during the partition process - only the amount of water present as a pure phase changes until it is all gone. This leads us to an important difference: in the partitioning of water in itself will always stay the same.

Can you calculate the partition constants that describe the air/water and octanol/water partition equilibrium of water at 25°C? The solubility of water in octanol is 2.3 mol/L and the equilibrium vapour pressure is 3169 Pa.

The equilibrium concentration of water in any other phase (at a given temperature) is also fix and does not depend on the total amount of the partitioning compound in the system. Therefore, the partition equilibrium of a chemical whose pure phase is part of the system can just as well be characterised by the respective equilibrium concentrations as by a

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partition constant.

 $K_{water air/water} = 2.36 E^{-5} [L_{water}/L_{air}]$ (to get to the result you need to use the gas law in order to transform the partial pressure into a concentration in mol_{water}/L_{air} and you need to know that water has a concentration of 55 mol/L in its liquid form.)

K_{water} octanol/water = 0.042 [L_{water} /L_{octanol}]

Note: Later, models will be presented that predict partition constants based on an estimation of the free energies of partitioning. These models work just as well for dilute solutes as they do for the partitioning of water out of its own phase into octanol for example. This is nice evidence that these partition processes are all governed by the same principals and that the differences in expressing the equilibrium state are only of formal nature.

2 b)

Could one also express solubility and vapor pressure in form of a partition constant?

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