# Ethyl acetate

You have an aquarium with 200 L of water. Above the aquarium you have installed a new lamp and while trying to remove the price tag with some ethyl acetate, you have spilled 10 ml of ethyl acetate into the aquarium. The water is well mixed and so you can assume that the ethyl acetate will be distributed evenly throughout the aquarium within minutes. Your air pump delivers 0.5 L/min (volume corresponds to atmospheric pressure) air to the water.

**a)** Which amount (in mol) ethyl acetate per minute would be removed from the water with the air bubbles assuming that a partition equilibrium between the water and the air bubbles is established? (Water and air have a temperature of 25°C.) Are your calculations based on any simplifying assumptions?

**b)** How does the answer look like if you had spilled 10 ml hexane instead of ethyl acetate? Can you proceed just like in the case of ethyl acetate and just fill in different numbers or are there principal differences?

In various literature sources you find the following properties:

**Ethyl acetate**

| | |
|---|---|
| Water solubility at 25 °C: | 0.90 mol/L |
| Saturation vapor pressure at 25 °C: | 12580 Pa |
| Measured Henry´s Law constant at 25 °C: | 17.1 Pa $m^3$ $mol^{-1}$ |
| Melting point: | -83.6 °C |
| Molecular weight: | 88.1 g/mol |
| Density at 25 °C: | 0.9 $g/cm^3$ |

**Hexane**

| | |
|---|---|
| Water solubility at 25 °C: | 1.5 $10^{-4}$ mol/L |
| Saturation vapor pressure at 25 °C: | 20130 Pa |

- Excercises for an improved intuitive understanding
- Questions for recapitulation
- Good to know
- Minesweeper-problems


| | |
|---|---|
| Measured Henry´s Law constant at 25 °C: | $1.63\ 10^{5}$ Pa $m^3$ $mol^{-1}$ |
| Melting point: | -95 °C |
| Molecular weight: | 86.2 g/mol |
| Density at 25 °C: | 0.66 $g/cm^3$ |

## Answer:

**a)** Concentration in water: 10 ml ethylacetate in 200 L water => 0.511 $mol/m^3$.
This corresponds to an equilibrium concentration in the air bubbles of => 8.73 Pa .
This amounts to (ideal gas law) : $3.52\ 10^{-3}$ mol $/m^3$.

Hence, at the beginning $1.76\ 10^{-6}$ mol per minute ethyl acetate are gassing out (= 0.15 mg / min). Of course, as time goes by this rate will decrease. The exact time curve for the outgassing process is described by an exponential curve, see text book chapter IX.1.1 (iv).

(Assumptions made: only bulk phase partitioning is relevant, i.e., there is no adsorption at the air –water interface; no sorption to other compartments such as fish, plants… , no direct outgassing at the water surface of the water, the compressability of the gas bubbles (at the bottom of the aquarium they will be smaller due to the pressure of the water column) is not accounted for.

**b)** No, you cannot proceed analogously because 10 ml of hexane will not completely dissolve in 200 L water. The aqueous concentration in this case would maximally correspond to the water solubility.