

Exercises solution

Master's degree in environmental science and engineering

Occupational and environmental health

2.1 Chemical pollutants - properties

1) Quiz question

a) Calculate the composition of the vapor phase in equilibrium with a mixture of 10% benzene and 90% xylene by volume

Benzene:

$$\rho_{20^{\circ}\text{C}} = 0.879 \text{ kg/l}$$

$$P^{\circ}_{\text{benzene}} (20^{\circ}\text{C}) = 10.0 \text{ kPa},$$

$$\text{MW} = 78.1 \text{ g/mol}$$

Xylene

$$\rho_{20^{\circ}\text{C}} = 0.864 \text{ kg/l}$$

$$P^{\circ}_{\text{xylene}} (20^{\circ}\text{C}) = 0.80 \text{ kPa}$$

$$\text{MW} = 106.2 \text{ g/mol}$$

The molar fraction of each product in the liquid mixture is determined:

$$m_{\text{benz}} = 0.1 \cdot 0.879 = 87.9 \text{ g}$$

$$\text{Nb. moles benzene} = 87.9/78.1 = 1.126 \text{ mol}$$

$$X_{\text{benz}} = 0.133$$

$$m_{\text{xyl}} = 0.9 \cdot 0.864 = 777.6 \text{ g}$$

$$\text{Nb. moles xylene} = 777.6/106.2 = 7.322 \text{ mol}$$

$$X_{\text{xyl}} = 0.867$$

The partial pressure corresponding to each of the substance becomes:

$$P_{\text{benz}} = 0.133 \cdot 10 = 1.33 \text{ kPa}$$

$$P_{\text{xyl}} = 0.867 \cdot 0.80 = 0.693 \text{ kPa}$$

There is about 2x more benzene than xylene in the vapor phase!

2) Blood concentration

The partition coefficient between blood and air at 37°C for benzene is 7.1. Calculate the concentration of benzene remaining in 1 ml of blood containing initially 5 mg/l, after equilibration with 10 ml of air at 37°C.

x = equilibrium blood benzene concentration [mg/l]

y = equilibrium air benzene concentration [mg/l]

the benzene in air at equilibrium [mg/l] is:

$$x/y = 7.1, \text{ hence } y = x/7.1$$

The total quantity ($5 \cdot 10^{-3}$ mg) is divided between the two phases:

$$5 \cdot 10^{-3} = x \cdot 10^{-3} + y \cdot 10 \cdot 10^{-3}$$

$$5 = x + 10 y = x + 10 x/7.1 = x (1 + 1.4)$$

$$\text{Thus, } x = 5/2.4 = 2.1 \text{ mg/l}$$

3) Surprise fridge

I am storing a mixture of 30% hexane and 70% non-flammable chlorinated solvent in a refrigerator at 4°C. Is there a risk of fire/explosion if there is a source of ignition (such as an electrical spark from the thermostat)?

The properties of hexane are as follows

Boiling point:	69°C
Melting point:	-95°C
Flash point:	-23°C
LEL:	1.2 %
UEL:	7.7 %
Vapor pressure (25°C):	256 mmHg
Vapor pressure (0°C):	~46 mmHg

- A. Yes, because the vapor pressure of the mixture exceeds the LEL at this temperature
- B. Yes, because the refrigerator temperature exceeds the flash point of hexane
- C. No, because the UEL is exceeded
- D. No, because the flash point of the mixture is higher than the refrigerator temperature

The temperature of the refrigerator being higher than the flash point of the product, we cannot exclude a priori the risk of fire. It must therefore be determined whether, under the most pessimistic conditions (at equilibrium), the concentrations of hexane vapor can exceed the lower flammability limits.

For simplicity, we consider a molar mixture of 30% hexane and we admit that the relation vapor pressure / temperature is linear between 0 and 25 °C.

Between 0 and 25 °C, the increase in vapor pressure (at saturation) is 8.4 mmHg/ °C.

The vapor pressure (at saturation) of hexane at 4°C becomes: $46 + 4 \times 8.4 = 79.6$ mmHg, or 10.6 kPa.

The partial pressure (at saturation) at equilibrium with the mixture becomes: $0.3 \times 10.6 = 3.18$ kPa, i.e. 3.13 % of the gas mixture. The LEL being exceeded, there is therefore a real risk of explosion of the refrigerator.

The correct answer is A. Answer B is incomplete because the flash point of the (pure) product is not sufficient in itself to explain the risk of explosion of the mixture.