Example Questions involving Gas Phase Concentrations

1. The National Institute of Occupational Safety and Health's recommended short-term (15 min) exposure limit for benzene (C_6H_6) is reported as 16.3 mg/m^3, whereas it's odour threshold is given 1.5 ppm$_v$.
a) If a benzene odour is detected, does this necessarily mean you have exceeded the short term expousure limit?
b) Benzene has a reported vapour pressure of 95.2 torr at 25°C. Calculate concentration of benzene in room air, if a large container of benzene was left open in a closed room. (Note; benzene is a known carcinogen, do not try this at home)

a) $16.3 \frac{mg}{m^3} \longrightarrow$ mole fraction (mixing ratio)

$$\text{mixing ratio} = \frac{n_{C_6H_6}}{n_{air}}$$

$n_{C_6H_6} \leftarrow 16.3 \frac{mg}{m^3} \times \frac{1\ mol}{78.2 g} \leftarrow MW_{C_6H_6} = 2.08 \times 10^{-4} \frac{mol}{m^3}$

$n_{air} \leftarrow \frac{P \cdot V}{R \cdot T} = \frac{(1.00\ atm)(10^3 L)}{(0.08206 \frac{L\,atm}{mol \cdot K})(298 K)} = 40.9 \frac{mol}{m^3}$

$$= \frac{2.08 \times 10^{-4}}{40.9} = 5.10 \times 10^{-6} \quad \text{or} \quad \boxed{5.10\ ppm_v}$$

b) $V.P. = 92.5\ torr \times \frac{1\ atm}{760\ torr} = 0.122\ atm \leftarrow P_{C_6H_6}$

If there is an inexhaustable supply of C_6H_6, and if there is enough time for the solution to equilibrate with the room air, then $P_{C_6H_6} = 0.122$ atm.

$$\text{mixing ratio} = \frac{n_{C_6H_6}}{n_{air}}$$

$n_{C_6H_6} \leftarrow P_{C_6H_6}(V/RT) = 4.98 \times 10^{-3}$ mols

$n_{air} \leftarrow P_{air}(V/RT) = 4.09 \times 10^{-2}$ mol.

$$= 0.122 \quad (\text{note } \chi_x = P_x/P_T)$$

$$\text{mass/volume} = \frac{n_{C_6H_6} \cdot MW}{V} = \frac{\frac{P \cdot V}{R \cdot T} \cdot MW}{V} = \frac{P \cdot MW}{RT}$$

$$= \frac{(0.122\ atm)(78.2\ g/mol)}{(0.08206 \frac{L \cdot atm}{mol/K})(298 K)} = 0.390\ g/L \quad \text{or} \quad \boxed{390\ g/m^3}$$

2. A student prepares a gas standard by injecting 86 mg of chloroform ($CHCl_3$) into a sealed 2.00L flask, whereupon it completely evaporates. Calculate the concentration of chloroform as ppm_v.

$$\text{mixing ratio} = \frac{n_{CHCl_3}}{n_{air}} = \frac{\text{mass}/MW}{PV/RT}$$

$$= \frac{86\ mg \times \frac{1\ mol}{119.5\ g} \times \frac{1\ g}{10^3\ mg}}{\frac{(1.00\ atm)(2.0\ L)}{(0.08206\ \frac{L\cdot atm}{mol/K})(298\ K)}}$$

$$= \frac{7.19\times10^{-4}}{0.0818} = 0.008791$$

or $\boxed{8790\ ppm_v}$

3. Calculate the number density of oxygen molecules in the atmosphere at an altitude of 30 km (0.015 atm, -40°C).

$$n^* = \frac{\#\text{molecules}}{cm^3}$$

$$n^*_{O_2}(30\ km) = \chi_{O_2}(30\ km) \times n^*_{air}(30\ km)$$

Taking $\chi_{O_2}(30km) = 0.21$

and $n^*_{air}(30km) = \frac{P\cdot V}{R\cdot T} \times N_A$

$$= \frac{(0.015\ atm)(10^{-3}L)(6.023\times10^{23}\ mol^{-1})}{(0.08206\ \frac{L\cdot atm}{mol\cdot K})(233\ K)}$$

$$= 4.72\times10^{17}\ \frac{molecules}{cm^3}$$

$\therefore n^*_{O_2}(30km) = (0.21)(4.72\times10^{17}\ molecules/cm^3)$

$= \boxed{1.0\times10^{17}\ molecules/cm^3}$

4. The average concentration of sulfur dioxide in Nikel Russia is 50 μg/m^3 at. What is the concentration of SO_2 in parts per billion at 15°C and 1 atm.

$$\text{mixing ratio} = \frac{n_{SO_2}}{n_{air}} = \frac{50\ \mu g/m^3 \times \frac{1\ mol}{64\ g} \times \frac{1\ g}{10^6\ \mu g}}{\frac{(1.00\ atm)(10^3\ L)}{(0.08206\ \frac{L \cdot atm}{mol/K})(288\ K)}}$$

$$= \frac{7.81 \times 10^{-7}}{42.3} = 1.8 \times 10^{-8}$$

OR ~~18~~ **18 ppbv**

5. If the mixing ratio of ozone in polluted urban air is 50 ppbv, calculate its concentration in mg m^{-3}.

$$\frac{mass}{m^3} \leftarrow \frac{50 \times 10^{-9}\ mols\ O_3}{1\ mol\ air} \times \frac{48\ g}{mol} \times \frac{10^3\ mg}{g} = \frac{0.0024\ mg}{mol\ air}$$

Volume of 1 mol air at $P = 1.0$ atm, $T = 288K$ is given by $V = \frac{nRT}{P}$

$$= \frac{(1.0\ mol)(0.08206\ \frac{L \cdot atm}{mol/K})(288\ K)}{(1.00\ atm)}$$

$$= 23.6\ L \quad \text{or} \quad 0.0236\ m^3$$

$$\therefore \frac{0.0024\ mg\ O_3}{0.0236\ m^3} = \boxed{0.10\ mg/m^3}$$