TDTS 25

Calculating atmospheric concentrations from analyte masses retained on sorbent tubes

It is recommended that this Application Note is read in conjunction with Application Note TDTS 7 (Calibration: Preparing and introducing thermal desorption standards using sorbent tubes).

Pumped monitoring

The relationship between atmospheric concentration and the mass of analyte in a volume of air is derived from Avogadro's law. The result of this, is that, at room temperature and pressure, the molar volume of the vapour of a pure compound is ~25 L mol^{-1}.

For example, at room temperature and pressure:

- 25 L of pure benzene vapour would contain 1 mol (78 g) of benzene
- 25 L of pure toluene vapour would contain 1 mol (92 g) of toluene

Calculations relating to analyte mass in a given volume of air, in terms of part per million (ppm) or part per billion (ppb) by volume, are therefore derived by considering the relative proportions as follows:

At room temperature and pressure:

- 25 L of air containing 1000 ppm (1 part in 1000) benzene would contain $^{1}/_{1000}$ mol (78 mg) of benzene
- 25 L of air containing 1000 ppm (1 part in 1000) toluene would contain $^{1}/_{1000}$ mol (92 mg) of toluene
- 10 L of air containing 10 ppb (1 part in 10^8) benzene would contain $(^{10}/_{25})\,(^{1}/_{10^8})$ mol (310 ng) of benzene
- 10 L of air containing 10 ppb (1 part in 10^8) toluene would contain $(^{10}/_{25})\,(^{1}/_{10^8})$ mol (370 ng) of toluene

...and so forth.

Reversing this calculation allows the calculation of the atmospheric concentration from the mass on the sorbent tube:

$$\text{Concentration (as a fraction)} = \frac{\text{Mass (g)}}{\text{Molar mass (g mol}^{-1})} \times \frac{25}{\text{Volume pumped onto tube (L)}} \qquad (1)$$

Therefore, if 10 L of air was pumped onto a sorbent tube and the mass of benzene collected was determined from GC(/MS) data to be 3.2 µg, the atmospheric concentration must have been:

$$\frac{3.2 \times 10^{-6}}{78} \times \frac{25}{10} = 1 \times 10^{-7} = 0.1 \text{ ppm}$$

Atmospheric concentration	Molar mass (g mol^{-1})				
	50	75	100	150	200
100 ppm	20 mg	30 mg	40 mg	60 mg	80 mg
10 ppm	200 µg	300 µg	400 µg	600 µg	800 µg
1 ppm	20 µg	30 µg	40 µg	60 µg	80 µg
10 ppb	200 ng	300 ng	400 ng	600 ng	800 ng
1 ppb	20 ng	30 ng	40 ng	60 ng	80 ng
100 ppt	2 ng	3 ng	4 ng	6 ng	8 ng

Table 1: Quick guide to analyte masses collected on a sorbent tube by pumped sampling of 10 L of air (at room temperature and pressure).

Diffusive monitoring

If diffusive sampling is working properly, a constant 'uptake rate' will be applicable to any given sorbent–analyte interaction (see Application Note TDTS 1 for a comprehensive listing). The general equation associated with diffusive samplers is:

$$\text{Mass sampled (collected)} = \text{Uptake rate} \times \text{Concentration} \times \text{Time}$$

Uptake rates (U) are typically quoted in ng ppm^{-1} min^{-1}. The mass collected on a sorbent tube can therefore be related to atmospheric concentration using the following equation:

$$U\ (\text{ng ppm}^{-1}\ \text{min}^{-1}) = \frac{\text{Mass (ng)}}{\text{Concentration (ppm)} \times \text{Time (min)}}$$

Or alternatively:

$$\text{Concentration (ppm)} = \frac{\text{Mass (ng)}}{U\ (\text{ng ppm}^{-1}\ \text{min}^{-1}) \times \text{Time (min)}} \qquad (2)$$

The units in these equations are suitable for workplace monitoring. However, for diffusive monitoring of ambient air, where concentrations are lower and sampling times longer, an alternative relationship is more convenient:

$$\text{Concentration (ppb)} = \frac{\text{Mass (ng)}}{10 \times U\ (\text{ng ppm}^{-1}\ \text{min}^{-1}) \times \text{Time (weeks)}}$$

Diffusive uptake rates are sometimes also quoted in mL min^{-1} for a pure sample of analyte. To derive an expression for conversion between the two units, one first needs to express the mass of a pure sample in terms of volume, as below:

$$\text{Mass (ng)} = \frac{\text{Molar mass (g mol}^{-1}) \times \text{Volume (nL)}}{\text{Molar volume (L mol}^{-1})}$$

Substitution of this into equation (2) and conversion of the volume from nL to mL then gives:

$$\text{Concentration (ppm)} = \frac{\text{Molar mass (g mol}^{-1}) \times \text{Volume (mL)} \times 10^6}{\text{Molar volume (L mol}^{-1}) \times U\ (\text{ng ppm}^{-1}\ \text{min}^{-1}) \times \text{Time (min)}}$$

Considering a pure sample (*i.e.* with a concentration of 10^6 ppm), rearrangement then gives:

$$\frac{\text{Volume (mL)}}{\text{Time (min)}} = \frac{\text{Molar volume (L mol}^{-1}) \times U\ (\text{ng ppm}^{-1}\ \text{min}^{-1})}{\text{Molar mass (g mol}^{-1})}$$

This results in the following equations for conversion between the two uptake rates:

$$U\ (\text{mL min}^{-1}) = \frac{\text{Molar volume (L mol}^{-1})}{\text{Molar mass (g mol}^{-1})} \times U\ (\text{ng ppm}^{-1}\ \text{min}^{-1})$$

and

$$U\ (\text{ng ppm}^{-1}\ \text{min}^{-1}) = \frac{\text{Molar mass (g mol}^{-1})}{\text{Molar volume (L mol}^{-1})} \times U\ (\text{mL min}^{-1})$$

The involvement of the molar volume in these expressions means that uptake rates given in mL min^{-1} are temperature-dependent, whereas those given in ng ppm^{-1} min^{-1} are temperature-independent.

Atmospheric concentration	Uptake rate (ng ppm^{-1} min^{-1})				
	1.3	**1.5**	**1.7**	**2.0**	**2.5**
100 ppm	0.624 mg	0.72 mg	0.816 mg	0.96 mg	1.2 mg
10 ppm	6.24 µg	7.2 µg	8.16 µg	9.6 µg	12.0 µg
1 ppm	0.624 µg	0.72 µg	0.816 µg	0.96 µg	1.2 µg
100 ppb	62.4 ng	72 ng	81.6 ng	96 ng	120 ng
10 ppb	6.24 ng	7.2 ng	8.16 ng	9.6 ng	12 ng
1 ppb	0.624 ng	0.72 ng	0.816 ng	0.96 ng	1.2 ng

Table 2: Quick guide to analyte masses collected on an axial sorbent tube by diffusive sampling over 8 h (at room temperature and pressure).

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