

*Note: the following are examples of the type of calculations you may be asked to perform in the TE3 narrative paper. Please note this is not a complete exam paper. Calculation questions typically make up 20 out of the 40 marks for the paper.*

## EXAMPLE CALCULATIONS ASSOCIATED WITH THE MEASUREMENT OF GASES AND VAPOURS USING MANUAL TECHNIQUES

### 1) To convert concentrations in ppm to mg/m<sup>3</sup>

CO concentration = 100 ppm  
Molecular weight of CO = 28  
Molar volume = 22.4 litres

$$\begin{aligned}\text{Concentration in mg/m}^3 &= \frac{\text{concentration (ppm)} \times \text{molecular weight of substance}}{\text{molar volume}} \\ &= \frac{100 \text{ ppm} \times 28}{22.4} \\ &= 125 \text{ mg/m}^3\end{aligned}$$

### 2) To convert concentrations in mg/m<sup>3</sup> to ppm

SO<sub>2</sub> concentration = 120 mg/m<sup>3</sup>  
Molecular weight of SO<sub>2</sub> = 64.07  
Molar volume = 22.4 litres

$$\begin{aligned}\text{Concentration in ppm} &= \frac{\text{concentration (mg/m}^3\text{)} \times \text{molar volume}}{\text{molecular weight of substance}} \\ &= \frac{120 \text{ mg/m}^3 \times 22.4}{64.07} \\ &= 42 \text{ ppm}\end{aligned}$$

### **3) To express total organic compounds (TOC) as carbon**

Toluene concentration = 50 mg/m<sup>3</sup>  
Molecular weight of toluene C<sub>7</sub>H<sub>8</sub> = 92  
Molecular weight of carbon = 12

TOC expressed as mg of carbon

$$\begin{aligned} &= \text{concentration of TOC compound} \times \frac{\text{mass of carbon in the molecule}}{\text{molecular weight of molecule}} \\ &= 50 \text{ mg/m}^3 \times (7 \times 12 / 92) \\ &= 45.7 \text{ mgC/m}^3 \end{aligned}$$

### **4) To express fluoride concentrations as hydrogen fluoride**

Fluoride concentration = 65 µgF/ml  
Molecular weight of fluoride, F = 19  
Molecular weight of hydrogen, H = 1  
Molecular weight of hydrogen fluoride HF = molecular weights of fluoride + hydrogen  
= 19 + 1  
= 20

$$\begin{aligned} \text{Fluoride to hydrogen fluoride correction factor} &= \frac{\text{molecular weight of HF}}{\text{molecular weight of F}} \\ &= \frac{20}{19} \\ &= 1.053 \end{aligned}$$

Fluoride expressed as hydrogen fluoride = fluoride concentration x 1.053

$$\begin{aligned} &= 65 \text{ µgF/ml} \times 1.053 \\ &= 68.4 \text{ µgHF/ml} \end{aligned}$$

### **5) To calculate the minimum sampling time required**

Concentration of compound in stack gas =  $2 \text{ mg/m}^3$  ( $2 \text{ } \mu\text{g/l}$ )

Sampling rate =  $2 \text{ l/min}$

Impinger solution volume =  $250 \text{ ml}$

Limit of detection (LOD) quoted by analytical laboratory =  $0.5 \text{ } \mu\text{g/ml}$

Rate of collection by sampling equipment

$$= \text{concentration of compound in stack gas} \times \text{sampling rate}$$

$$= 2 \text{ } \mu\text{g/l} \times 2 \text{ l/min}$$

$$= 4 \text{ } \mu\text{g/min}$$

Target mass of compound required

$$= \text{impinger solution volume} \times \text{LOD}$$

$$= 250 \text{ ml} \times 0.5 \text{ } \mu\text{g/ml}$$

$$= 125 \text{ } \mu\text{g}$$

Minimum sampling time required

$$= \frac{\text{target mass of compound}}{\text{rate of collection}}$$

$$= \frac{125 \text{ } \mu\text{g}}{4 \text{ } \mu\text{g/min}}$$

$$= 31 \text{ minutes}$$

## 6) To calculate the percentage by volume of moisture in a duct

In this example it is assumed that moisture is collected in accordance with BS EN 14790:2005. The sampling equipment utilises two impingers containing water, and one impinger containing silica gel.

Initial meter reading = 6.291 m<sup>3</sup>  
 Final meter reading = 6.351 m<sup>3</sup>  
 Molecular weight of moisture, H<sub>2</sub>O = 18  
 Molar volume at STP = 22.4 litres  
 Mass of moisture collected in impinger 1 = 3.2g  
 Mass of moisture collected in impinger 2 = 1.3g  
 Mass of moisture collected in silica gel = 0.7g  
 Dry gas meter pressure = 100.7 kPa  
 Dry gas meter temperature = 16°C  
 Standard temperature = 273 K  
 Standard pressure = 101.3 kPa

### 6.1 Calculate the sample volume at the dry gas meter

Initial meter reading = 6.291 m<sup>3</sup>  
 Final meter reading = 6.351 m<sup>3</sup>

$$\begin{aligned}\text{Sample volume at dry gas meter} &= \text{final reading} - \text{initial reading} \\ &= 6.351 \text{ m}^3 - 6.291 \text{ m}^3 \\ &= 0.06 \text{ m}^3 \text{ (60 litres)}\end{aligned}$$

### 6.2 Correct the sampled gas volume to standard conditions

Dry gas meter sampled volume corrected to STP

$$\begin{aligned}&= \text{sampled volume} \times \frac{\text{standard temperature}}{\text{temperature at dry gas meter}} \times \frac{\text{dry gas meter pressure}}{\text{standard pressure}} \\ &= 60 \text{ litres} \times \frac{273 \text{ K}}{273 + 16 \text{ K}} \times \frac{100.7 \text{ kPa}}{101.3 \text{ kPa}} \\ &= 60 \text{ litres} \times 0.94 \times 0.99 \\ &= 55.8 \text{ litres}\end{aligned}$$

### 6.3 Calculate the total mass of moisture collected

$$\begin{aligned}\text{Total mass of moisture} &= \text{mass in impinger 1} + \text{mass in impinger 2} + \text{mass in silica gel} \\ &= 3.2 \text{ g} + 1.3 \text{ g} + 0.7 \text{ g} \\ &= 5.2 \text{ g}\end{aligned}$$

**6.4 Calculate the volume of collected moisture at STP**

$$\begin{aligned}\text{Volume of collected moisture} &= \frac{\text{total moisture collected} \times \text{molar volume}}{\text{molecular weight of H}_2\text{O}} \\ &= \frac{5.2 \text{ g} \times 22.4}{18} \\ &= 6.47 \text{ litres}\end{aligned}$$

**6.5 Calculate the percentage by volume of moisture**

$$\begin{aligned}\text{Percentage of moisture} &= \frac{\text{volume of moisture collected}}{\text{total volume of dry gas and moisture}} \times 100 \\ &= \frac{6.47 \text{ litres}}{55.8 + 6.47 \text{ litres}} \times 100 \\ &= 10.4 \%\end{aligned}$$

## **7. To calculate the concentration of a substance in a stack gas from the analytical laboratory results**

Analysis of solution for impinger 1 = 23.6 µg/ml  
Analysis of solution for impinger 2 = 0.8 µg/ml  
Volume of sample solution from impinger 1 = 260 ml  
Volume of sample solution from impinger 2 = 240 ml  
Sampled gas volume at STP = 350 litres

### **7.1 Calculate the total mass of the substance recovered**

Mass of substance from impinger 1

$$\begin{aligned} &= \text{volume of sample solution from impinger 1} \times \text{concentration of substance} \\ &= 260 \text{ ml} \times 23.6 \text{ µg/ml} \\ &= 6136 \text{ µg} \end{aligned}$$

Mass of substance from impinger 2

$$\begin{aligned} &= \text{volume of sample solution from impinger 2} \times \text{concentration of substance} \\ &= 240 \text{ ml} \times 0.8 \text{ µg/ml} \\ &= 192 \text{ µg} \end{aligned}$$

Total mass of substance collected in mg

$$\begin{aligned} &= \frac{\text{mass of substance from impinger 1} + \text{mass of substance from impinger 2}}{1000} \\ &= \frac{6136 \text{ µg} + 192 \text{ µg}}{1000} \\ &= 6.33 \text{ mg} \end{aligned}$$

### **7.2 Calculate the concentration of the substance in the stack**

$$\begin{aligned} \text{Concentration of substance in the stack} &= \frac{\text{total mass of substance collected}}{\text{sampled gas volume at STP}} \times 1000 \\ &= \frac{6.33 \text{ mg}}{350 \text{ litres}} \times 1000 \\ &= 18.1 \text{ mg/m}^3 \end{aligned}$$

Note: multiply by 1000 to convert from litres to m<sup>3</sup>, as 1m<sup>3</sup> = 1000 litres

### **7.3 Calculate and assess the impinger absorption solution collection efficiency**

Mass of substance from impinger 1 = 6.14 mg

Mass of substance from impinger 2 = 0.19 mg

Total mass of substance collected

= mass of substance from impinger 1 + mass of substance from impinger 2

= 6.14 mg + 0.19 mg

= 6.33 mg

Impinger efficiency

=  $\frac{\text{mass of substance from impinger 1}}{\text{total mass of substance from both impingers}} \times 100$

=  $\frac{6.14 \text{ mg}}{6.33 \text{ mg}} \times 100$

= 97%

The impinger efficiency is acceptable as it is greater than 95%

## 8. To calculate mass emissions to atmosphere

Total mass of substance collected during sampling = 730 µg

Sample gas volume at STP, dry = 8.5 litres

Stack cross section area, CSA = 1.1 m<sup>2</sup>

Average stack gas velocity = 10.4 m/s

Temperature of stack gas = 62 °C

Pressure in stack = 101.3 kPa

Moisture content of stack gas = 7%

### 8.1 Calculate the concentration of the substance at STP, dry

Concentration of substance at STP, dry

$$= \frac{\text{mass of substance collected}}{\text{sample gas volume at STP, dry}}$$

$$= \frac{730 \text{ µg}}{8.5 \text{ litres}}$$

$$= 85.9 \text{ µg/l (85.9 mg/m}^3\text{)}$$

### 8.2 Calculate the concentration of the substance at stack gas conditions

Stack temperature is 62 °C

Stack pressure is 101.3 kPa

Stack moisture is 7%

Reference pressure is 101.3 kPa

Reference moisture is dry

$$\text{Temperature correction factor} = \frac{\text{standard temperature}}{\text{stack temperature}}$$

$$= \frac{273 \text{ K}}{273 + 62 \text{ K}}$$

$$= 0.815$$

$$\text{Moisture correction factor} = \frac{(100 - \text{stack moisture})}{100}$$

$$= \frac{(100 - 7)}{100}$$

$$= 0.93$$

A correction for pressure is not required in this situation as the stack pressure is the same as the reference pressure.



Concentration of substance at stack conditions

$$\begin{aligned} &= \text{Concentration as measured} \times \text{correction factor for temperature} \times \\ &\quad \text{correction factor for moisture} \\ &= 85.9 \text{ mg/m}^3 \times 0.815 \times 0.93 \\ &= 65.1 \text{ mg/m}^3 \end{aligned}$$

### **8.3 Calculate the volume flow in the stack**

Average stack gas velocity = 10.4 m/s  
Stack cross section area, CSA = 1.1 m<sup>2</sup>  
Seconds in 1 hour = 3600

$$\begin{aligned} \text{Volume flow rate in m}^3/\text{s} &= \text{average gas velocity in m/s} \times \text{stack cross section area} \\ &= 10.4 \text{ m/s} \times 1.1 \text{ m}^2 \\ &= 11.44 \text{ m}^3/\text{s} \end{aligned}$$

$$\begin{aligned} \text{Volume flow rate in m}^3/\text{h} &= \text{volume flow rate in m}^3/\text{s} \times \text{seconds in 1 hour} \\ &= 11.4 \text{ m}^3/\text{s} \times 3600 \\ &= 41184 \text{ m}^3/\text{hr} \end{aligned}$$

### **8.4 Calculate the mass emission to atmosphere in g/hr**

$$\begin{aligned} \text{Mass emission rate} &= \frac{\text{volume flow rate in the stack} \times \text{concentration of substance}}{1000} \\ &= 41184 \text{ m}^3/\text{hr} \times 65.1 \text{ mg/m}^3 \\ &= \frac{2681078 \text{ mg/hr}}{1000} \\ &= 2681 \text{ g/hr} \end{aligned}$$

## **9. To calculate the sampling time for a method using adsorption tubes**

Preferred sampling rate = 0.4 l/min

Concentration of substance in the stack = 17 mg/m<sup>3</sup> (17 µg/l)

Detection limit = 1.3 µg/l

Mass of collected sample to be 50 times the limit of detection limit (LOD)

$$\begin{aligned}\text{Mass of substance required in sample} &= 50 \times \text{LOD} \\ &= 50 \times 1.3 \mu\text{g/l} \\ &= 65 \mu\text{g}\end{aligned}$$

$$\begin{aligned}\text{Sample volume required} &= \frac{\text{mass of substance required in sample}}{\text{concentration of substance in the stack}} \\ &= \frac{65 \mu\text{g}}{17 \mu\text{g/l}} \\ &= 3.8 \text{ litres}\end{aligned}$$

$$\begin{aligned}\text{Minimum sampling time required} &= \frac{\text{sample volume required}}{\text{sampling rate}} \\ &= \frac{3.8 \text{ litres}}{0.4 \text{ l/min}} \\ &= 9.5 \text{ minutes}\end{aligned}$$

**10. To calculate the minimum detectable concentration in the stack at the given sampling rate.**

Actual sampling time = 15 minutes

Sampling rate = 0.4 l/min

Detection limit = 1 µg

Sampling volume achieved in 15 minutes = sampling time x sampling rate

$$= 15 \text{ minutes} \times 0.4 \text{ l/min}$$

$$= 6 \text{ litres}$$

Detection limit = 1 µg (0.001 mg)

Sampling volume = 6 litres (0.006 m<sup>3</sup>)

Minimum detectable concentration = 1 µg in 6 litres

Minimum detectable concentration per m<sup>3</sup> =  $\frac{1 \text{ µg}}{6 \text{ litres}}$

$$= 0.17 \text{ µg/l}$$

$$= 0.17 \text{ mg/m}^3$$