

*Note: the following are examples of the type of calculations you may be asked to perform in the TE4 narrative paper. This is not a complete exam paper. Calculation questions typically make up 20 out of 40 marks for a paper.*

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

### **1 To calculate total NO<sub>x</sub> in mg/m<sup>3</sup> at reference conditions given NO and NO<sub>2</sub> measurements in ppm**

NO concentration = 34 ppm (dry)  
NO<sub>2</sub> concentration = 15 ppm (dry)  
Measured oxygen level = 12%  
Reference conditions = STP, 15% O<sub>2</sub>, dry  
Atomic weight of N = 14  
Atomic weight of O = 16  
Molar volume = 22.4 litres

#### **1.1 To calculate the total NO<sub>x</sub> concentration in ppm**

$$\begin{aligned}\text{Total NO}_x \text{ concentration} &= \text{NO concentration} + \text{NO}_2 \text{ concentration} \\ &= 34 \text{ ppm} + 15 \text{ ppm} \\ &= 49 \text{ ppm}\end{aligned}$$

#### **1.2 To calculate the molecular weight of NO<sub>x</sub> as NO<sub>2</sub>**

$$\begin{aligned}\text{Molecular weight of NO}_2 &= \text{atomic weight of N} + \text{molecular weight of O}_2 \\ &= 14 + (16 \times 2) \\ &= 46\end{aligned}$$

#### **1.3 To convert NO<sub>x</sub> concentrations in ppm to NO<sub>2</sub> in mg/m<sup>3</sup>**

NO<sub>x</sub> concentration = 49 ppm  
Molecular weight of NO<sub>2</sub> = 46  
Molar volume = 22.4 litres

$$\begin{aligned}\text{Concentration in mg/m}^3 &= \frac{\text{concentration (ppm)} \times \text{molecular weight of substance}}{\text{molar volume}} \\ &= \frac{49 \text{ ppm} \times 46}{22.4} \\ &= 100.6 \text{ mg/m}^3\end{aligned}$$

#### 1.4 To calculate the concentration of NO<sub>2</sub> at reference conditions

Measured oxygen level = 12%

Reference oxygen = 15%

$$\begin{aligned}\text{Oxygen correction factor} &= \frac{(21 - \text{reference oxygen})}{(21 - \text{measured oxygen})} \\ &= \frac{(21 - 15)}{(21 - 12)} \\ &= 0.67\end{aligned}$$

Concentration at reference conditions

$$\begin{aligned}&= \text{Concentration as measured} \times \text{correction factor for oxygen} \\ &= 100.6 \text{ mg/m}^3 \times 0.67 \\ &= 67.4 \text{ mg/m}^3\end{aligned}$$

#### 2 To calculate concentrations at reference conditions in mg/m<sup>3</sup> from analyser results in ppm

Concentration of substance = 120 ppm

Measured moisture level = 9%

Reference moisture is dry

Measured oxygen level = 12.5% (wet)

Reference oxygen = 11%

Molecular weight of substance = 28

Molar volume = 22.4 litres

(In this example the molecule is CO)

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

Concentration of substance = 120 ppm

Molecular weight of substance = 28

Molar volume = 22.4 litres

$$\begin{aligned}\text{Concentration in mg/m}^3 &= \frac{\text{concentration (ppm)} \times \text{molecular weight of substance}}{\text{molar volume}} \\ &= \frac{120 \text{ ppm} \times 28}{22.4} \\ &= 150 \text{ mg/m}^3\end{aligned}$$

**2.2 To calculate the concentration of a substance at reference conditions**

$$\begin{aligned}\text{Moisture correction factor} &= \frac{100}{(100 - \text{measured moisture})} \\ &= \frac{100}{(100 - 9)} \\ &= 1.1\end{aligned}$$

(Note that the oxygen was measured on a wet basis and should be corrected to dry conditions)

$$\begin{aligned}\text{Oxygen at reference conditions} &= \text{measured oxygen} \times \text{correction factor for moisture} \\ &= 12.5\% \times 1.1 \\ &= 13.8\% \text{ (dry)}\end{aligned}$$

$$\begin{aligned}\text{Oxygen correction factor} &= \frac{(21 - \text{reference oxygen})}{(21 - \text{measured oxygen, dry})} \\ &= \frac{(21 - 11)}{(21 - 13.8)} \\ &= 1.4\end{aligned}$$

Concentration of substance at reference conditions

$$\begin{aligned}&= \text{concentration as measured} \times \text{correction factor for oxygen} \times \\ &\quad \text{correction factor for moisture} \\ &= 150 \text{ mg/m}^3 \times 1.4 \times 1.1 \\ &= 231 \text{ mg/m}^3\end{aligned}$$

**3 To express analyser readings in ppm (wet) at reference conditions in mg/m<sup>3</sup> (dry)**

NO<sub>x</sub> concentration = 80 ppm (wet)  
Measured moisture level = 10%  
Molar volume at STP = 22.4 litres  
Atomic weight of N = 14  
Atomic weight of O = 16

**3.1 To calculate the molecular weight of NO<sub>2</sub>**

Molecular weight of NO<sub>2</sub> = atomic weight of N + molecular weight of O<sub>2</sub>  
$$= 14 + (16 \times 2)$$
$$= 46$$

**3.2 To convert concentration in ppm to mg/m<sup>3</sup>**

Concentration in mg/m<sup>3</sup> =  $\frac{\text{concentration (ppm)} \times \text{molecular weight of substance}}{\text{molar volume}}$   
$$= \frac{80 \text{ ppm} \times 46}{22.4}$$
$$= 164 \text{ mg/Nm}^3 \text{ (wet)}$$

**3.3 To calculate the concentration at reference conditions dry**

Moisture correction factor =  $\frac{100}{(100 - \text{measured moisture})}$   
$$= \frac{100}{100 - 10}$$
$$= 1.1$$

NO<sub>2</sub> concentration (dry)

= concentration as measured x correction factor for moisture  
$$= 164 \text{ mg/Nm}^3 \times 1.1$$
$$= 180 \text{ mg/Nm}^3 \text{ (dry)}$$

**4 To calculate a mass emission rate in kg/h (Example 1)**

Volume flow rate at STP (wet) = 43 Nm<sup>3</sup>/s

NO<sub>2</sub> concentration (wet) = 164 mg/m<sup>3</sup>

Seconds in 1 hour = 3600

**4.1 To calculate the volume flow in the stack**

$$\begin{aligned}\text{Volume flow rate in Nm}^3/\text{h} &= \text{volume flow rate in Nm}^3/\text{s} \times \text{seconds in 1 hour} \\ &= 43 \text{ Nm}^3/\text{s} \times 3600 \\ &= 154,800 \text{ Nm}^3/\text{h}\end{aligned}$$

**4.2 To calculate the mass emission to atmosphere in kg/h**

$$\begin{aligned}\text{Mass emission rate in kg/h} &= \frac{\text{volume flow rate m}^3/\text{h} \times \text{concentration in mg/m}^3}{1 \times 10^6} \\ &= \frac{154,800 \text{ Nm}^3/\text{h} \times 164 \text{ mg/m}^3}{1 \times 10^6} \\ &= 25.4 \text{ kg/h}\end{aligned}$$

(Note dividing by 1 x 10<sup>6</sup> converts the result from mg to kg)

**5 To calculate a mass emission in kg/h (Example 2)**

Average stack gas velocity = 10 m/s

Stack diameter = 0.9 m (radius = 0.45 m)

Concentration of substance = 150 mg/m<sup>3</sup> (measured wet with no correction for oxygen or temperature)

**5.1 To calculate the cross section area of the stack**

$$\begin{aligned}\text{Cross sectional area of stack} &= \pi r^2 \\ &= 3.14 \times 0.45^2 \\ &= 0.64 \text{ m}^2\end{aligned}$$

**5.2 To calculate the volume flow in the stack**

$$\begin{aligned}\text{Volume flow rate in m}^3/\text{s} &= \text{cross section area of stack} \times \text{average gas velocity} \\ &= 0.64 \text{ m}^2 \times 10 \text{ m/s} \\ &= 6.4 \text{ m}^3/\text{s}\end{aligned}$$

$$\begin{aligned}\text{Volume flow rate in m}^3/\text{h} &= \text{volume flow rate in m}^3/\text{s} \times \text{seconds in 1 hour} \\ &= 6.4 \text{ m}^3/\text{s} \times 3600 \\ &= 23,040 \text{ m}^3/\text{h}\end{aligned}$$

**5.3 To calculate the mass emission in kg/h at stack conditions**

$$\begin{aligned}\text{Mass emission} &= \frac{\text{volume flow rate} \times \text{concentration of substance}}{1 \times 10^6} \\ &= \frac{23,040 \text{ m}^3/\text{h} \times 150 \text{ mg}/\text{m}^3}{1 \times 10^6} \\ &= 3.46 \text{ kg/h}\end{aligned}$$

(Note dividing by  $1 \times 10^6$  converts the result from mg to kg)

**6 To convert VOC results from a FID analyser to reference conditions**

VOC concentration = 23 mgC/m<sup>3</sup>  
Measured moisture level = 9.5%  
Reference moisture is dry  
Measured oxygen level = 13.2% (dry)  
Reference oxygen = 11%

(Note that the FID analyser measures hot and wet)

$$\begin{aligned}\text{Oxygen correction factor} &= \frac{(21 - \text{reference oxygen})}{(21 - \text{measured oxygen})} \\ &= \frac{(21 - 11)}{(21 - 13.2)} \\ &= 1.3\end{aligned}$$

$$\begin{aligned}\text{Moisture correction factor} &= \frac{100}{(100 - \text{measured moisture})} \\ &= \frac{100}{(100 - 9.5)} \\ &= 1.1\end{aligned}$$

Concentration at reference conditions

$$\begin{aligned}&= \text{Concentration as measured} \times \text{correction factor for oxygen} \times \text{correction factor for moisture} \\ &= 23 \text{ mgC}/\text{m}^3 \times 1.3 \times 1.1 \\ &= 33 \text{ mgC}/\text{m}^3\end{aligned}$$

**7 To calculate the concentration of VOCs as Carbon (C) as a dry gas and calculate the mass emissions of carbon and toluene from the results provided by a FID analyser**

VOC concentration = 185 ppm (propane equivalent  $C_3H_8$ )

Measured moisture level = 6.5%

Atomic weight of C = 12

Atomic weight of H = 1

Molar volume at STP = 22.4 litres

Stack gas flow rate =  $0.4 \text{ m}^3/\text{s}$

**7.1 To calculate the molecular weight of propane as carbon**

Molecular weight of propane as carbon

$$= \text{number of carbon atoms in molecule} \times \text{atomic weight of carbon}$$

$$= 3 \times 12$$

$$= 36$$

**7.2 To calculate the concentration of VOC in mgC at STP wet**

$$= \frac{\text{concentration in ppm} \times \text{molecular weight of propane as carbon}}{\text{molar volume}}$$

$$= \frac{185 \text{ ppm} \times 36}{22.4}$$

$$= 297 \text{ mgC/Nm}^3$$

**7.3 To calculate the concentration of VOC in mgC as a dry gas**

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

$$= \frac{100}{100 - 6.5}$$

$$= 1.07$$

$$\text{Concentration of VOC(dry)} = \text{VOC concentration wet} \times \text{correction factor for moisture}$$

$$= 297 \text{ mgC/Nm}^3 \times 1.07$$

$$= 318 \text{ mgC/Nm}^3$$

**7.4 To calculate the hourly emission rate in gC/h**

Stack gas flow rate = 0.4 m<sup>3</sup>/s

Concentration of VOC = 297 mgC/Nm<sup>3</sup> (wet)

$$\begin{aligned}\text{Volume flow rate in m}^3/\text{h} &= \text{flow rate in m}^3/\text{s} \times \text{seconds in 1 hour} \\ &= 0.4 \text{ m}^3/\text{s} \times 3600 \\ &= 1440 \text{ m}^3/\text{h}\end{aligned}$$

$$\begin{aligned}\text{Mass emission rate g/h} &= \frac{\text{volume flow rate m}^3/\text{h} \times \text{concentration of substance}}{1000} \\ &= \frac{1440 \text{ m}^3/\text{h} \times 297 \text{ mgC/Nm}^3}{1000} \\ &= 428 \text{ gC/h}\end{aligned}$$

(Note dividing by 1000 converts the result from mg to g)

**7.5 To calculate the mass emission as g toluene per hour**

Toluene = C<sub>7</sub>H<sub>8</sub>

Molecular weight of toluene as mgC

$$\begin{aligned}&= \text{number of carbon atoms in molecule} \times \text{atomic weight of carbon} \\ &= 7 \times 12 \\ &= 84\end{aligned}$$

Molecular weight of toluene

$$\begin{aligned}&= (\text{number of carbon atoms} \times \text{molecular weight of carbon}) + \\ &\quad (\text{number of hydrogen atoms} \times \text{atomic weight of hydrogen}) \\ &= (7 \times 12) + (8 \times 1) \\ &= 92\end{aligned}$$

Ratio of molecular weight of toluene to molecular weight of toluene as carbon

$$\begin{aligned}&= \frac{\text{molecular weight of toluene}}{\text{molecular weight of toluene as carbon}} \\ &= \frac{92}{84} \\ &= 1.095\end{aligned}$$

Mass emission expressed as gT/h

= mass emission rate gC/h x toluene to carbon mass ratio

= 428 gC/h x 1.095

= 469 gT/h

## **8 To calculate an uncertainty budget**

The performance characteristics of the analyser are as follows:

Type

B Sensitivity to ambient temperature = 1.5% of the certified range per 10K of variation

B Sensitivity to atmospheric pressure = 0.7% of the certified range per kPa

B Uncertainty of calibration gas = 1.5%

A Standard deviation of repeatability at span = 0.9% of the certified range

Certification range of analyser = 0 – 175 mg/m<sup>3</sup>

Maximum ambient temperature variation during sampling = 8K (± 4K relative to the temperature value at calibration)\*

Ambient pressure range during sampling = 98.8 – 101.2 kPa (± 1.2 kPa relative to a pressure value of 100 kPa at calibration)\*

Calibration gas concentration = 140 mg/m<sup>3</sup>

\* Note : The exams will not require a calculation of an uncertainty where the variation is not symmetrical about the value at calibration

### **8.1 To calculate the standard uncertainty in mg/m<sup>3</sup> associated with the ambient temperature variations**

Sensitivity of analyser to ambient temperature variations = 1.5% of the certified range per 10K of variation

Certification range = 0 – 175 mg/m<sup>3</sup>

Maximum ambient temperature variation during sampling = ± 4 K

### **8.2 To calculate the sensitivity per degree of ambient temperature change**

=  $\frac{\text{certified range} \times \text{sensitivity}}{10 \text{ K}}$

=  $\frac{175 \text{ mg/m}^3 \times 0.015}{10\text{K}}$

= 0.26 mg/m<sup>3</sup> per degree

**8.3 To calculate the standard uncertainty associated with the ambient temperature variation**

Standard uncertainty  $U_{temp}$

$$\begin{aligned} &= \frac{\text{sensitivity per degree} \times \text{variation in ambient temperature}}{\sqrt{3}} \\ &= \frac{0.26 \text{ mg/m}^3 \times 4 \text{ K}}{\sqrt{3}} \\ &= 0.6 \text{ mg/m}^3 \end{aligned}$$

**8.4 To calculate the standard uncertainty in  $\text{mg/m}^3$  associated with ambient pressure changes**

Sensitivity of analyser to ambient pressure variations = 0.7% of the certified range per kPa of pressure change

Certification range =  $175 \text{ mg/m}^3$

Ambient pressure range during sampling = 98.8 – 101.2 kPa

$$\begin{aligned} \text{Variation in ambient pressure} &= \frac{101.2 - 98.8}{2} \\ &= \pm 1.2 \text{ kPa} \end{aligned}$$

$$\begin{aligned} \text{Sensitivity per kPa of pressure change} &= \text{certification range} \times \text{sensitivity} \\ &= 175 \text{ mg/m}^3 \times 0.007 \\ &= 1.23 \text{ mg/m}^3 \text{ per kPa} \end{aligned}$$

Standard uncertainty associated with ambient pressure changes  $U_{apress}$

$$\begin{aligned} &= \frac{\text{sensitivity} \times \text{variation in ambient pressure}}{\sqrt{3}} \\ &= \frac{1.23 \text{ mg/m}^3 \times 1.2 \text{ kPa}}{\sqrt{3}} \\ &= 0.85 \text{ mg/m}^3 \end{aligned}$$

**8.5 To calculate the standard uncertainty of the calibration gas in  $\text{mg/m}^3$**

Uncertainty of calibration gas = 1.5%

Calibration gas value =  $140 \text{ mg/m}^3$

Standard uncertainty of calibration gas  $U_{cal}$

$$= \frac{\text{calibrated gas value} \times \text{uncertainty of calibration gas}}{\sqrt{3}}$$

$$= \frac{140 \text{ mg/m}^3 \times 0.015}{\sqrt{3}}$$

$$= 1.21 \text{ mg/m}^3$$

**8.6 To calculate the standard deviation of repeatability at span level in mg/m<sup>3</sup>**

Standard deviation of repeatability at span level = 0.9% of the certified range (note that this is a 'Type A' uncertainty and does not need to be divided by  $\sqrt{3}$ )

Certified range of analyser = 175 mg/m<sup>3</sup>

Standard deviation of repeatability at span  $U_{s,r}$

= certified range x standard deviation of repeatability at span

$$= 175 \text{ mg/m}^3 \times 0.9\%$$

$$= 1.58 \text{ mg/m}^3$$

**8.7 To calculate the combined standard uncertainty**

$$\begin{aligned} \text{Combined uncertainty} &= \sqrt{U_{\text{temp}}^2 + U_{\text{apress}}^2 + U_{\text{cal}}^2 + U_{s,r}^2} \\ &= \sqrt{0.6^2 + 0.85^2 + 1.21^2 + 1.58^2} \\ &= \sqrt{0.36 + 0.72 + 1.46 + 2.5} \\ &= 2.25 \text{ mg/m}^3 \end{aligned}$$

Expanded uncertainty = combined uncertainty x 1.96

$$= 2.05 \text{ mg/m}^3 \times 1.96$$

$$= 4.4 \text{ mg/m}^3$$