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

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

1) To convert concentrations in ppm to mg/m^3

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

$$\text{Concentration in mg/m}^3 = \frac{\text{concentration (ppm)} \times \text{molecular weight of substance}}{\text{molar volume}}$$

$$= \frac{100\ \text{ppm} \times 28}{22.4}$$

$$= 125\ \text{mg/m}^3$$

2) To convert concentrations in mg/m^3 to ppm

SO_2 concentration = 120 mg/m^3
Molecular weight of SO_2 = 64.07
Molar volume = 22.4 litres

$$\text{Concentration in ppm} = \frac{\text{concentration (mg/m}^3\text{)} \times \text{molar volume}}{\text{molecular weight of substance}}$$

$$= \frac{120\ \text{mg/m}^3 \times 22.4}{64.07}$$

$$= 42\ \text{ppm}$$

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

Toluene concentration = 50 mg/m^3
Molecular weight of toluene C_7H_8 = 92
Molecular weight of carbon = 12

TOC expressed as mg of carbon

$$= \text{concentration of TOC compound} \times \frac{\text{mass of carbon in the molecule}}{\text{molecular weight of molecule}}$$

= 50 mg/m^3 x (7 x 12 / 92)

= 45.7 mgC/m^3

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

Fluoride to hydrogen fluoride correction factor $= \frac{\text{molecular weight of HF}}{\text{molecular weight of F}}$

$= \frac{20}{19}$

= 1.053

Fluoride expressed as hydrogen fluoride = fluoride concentration x 1.053

= 65 µgF/ml x 1.053

= 68.4 µgHF/ml

5) To calculate the minimum sampling time required

Concentration of compound in stack gas = 2 mg/m^3 (2 µg/l)
Sampling rate = 2 l/min
Impinger solution volume = 250 ml
Limit of detection (LOD) quoted by analytical laboratory = 0.5 µg/ml

Rate of collection by sampling equipment

= concentration of compound in stack gas x sampling rate

= 2 µg/l x 2 l/min

= 4 µg/min

Target mass of compound required

= impinger solution volume x LOD

= 250 ml x 0.5 µg/ml

= 125 µg

Minimum sampling time required

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

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

= 31 minutes

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

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^3
Final meter reading = 6.351 m^3
Molecular weight of moisture, H_2O = 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^{o}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^3
Final meter reading = 6.351 m^3

Sample volume at dry gas meter = final reading – initial reading

$$= 6.351\ m^3 - 6.291\ m^3$$

$$= 0.06\ m^3\ \text{(60 litres)}$$

6.2 Correct the sampled gas volume to standard conditions

Dry gas meter sampled volume corrected to STP

$$= \text{sampled volume} \times \frac{\text{standard temperature}}{\text{temperature at dry gas meter}} \times \frac{\text{dry gas meter pressure}}{\text{standard pressure}}$$

$$= 60\ \text{litres} \times \frac{273\ \text{K}}{273 + 16\ \text{K}} \times \frac{100.7\ \text{kPa}}{101.3\ \text{kPa}}$$

$$= 60\ \text{litres} \times 0.94 \times 0.99$$

$$= 55.8\ \text{litres}$$

6.3 Calculate the total mass of moisture collected

Total mass of moisture = mass in impinger 1 + mass in impinger 2 + mass in silica gel

$$= 3.2\ g + 1.3\ g + 0.7\ g$$

$$= 5.2\ g$$

6.4 Calculate the volume of collected moisture at STP

$$\text{Volume of collected moisture} = \frac{\text{total moisture collected} \times \text{molar volume}}{\text{molecular weight of } H_2O}$$

$$= \frac{5.2\ \text{g} \times 22.4}{18}$$

$$= 6.47\ \text{litres}$$

6.5 Calculate the percentage by volume of moisture

$$\text{Percentage of moisture} = \frac{\text{volume of moisture collected}}{\text{total volume of dry gas and moisture}} \times 100$$

$$= \frac{6.47\ \text{litres}}{55.8 + 6.47\ \text{litres}} \times 100$$

$$= 10.4\ \%$$

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

= volume of sample solution from impinger 1 x concentration of substance

= 260 ml x 23.6 µg/ml

= 6136 µg

Mass of substance from impinger 2

= volume of sample solution from impinger 2 x concentration of substance

= 240 ml x 0.8 µg/ml

= 192 µg

Total mass of substance collected in mg

$$= \frac{\text{mass of substance from impinger 1 + mass of substance from impinger 2}}{1000}$$

$$= \frac{6136\ \mu g + 192\ \mu g}{1000}$$

= 6.33 mg

7.2 Calculate the concentration of the substance in the stack

$$\text{Concentration of substance in the stack} = \frac{\text{total mass of substance collected}}{\text{sampled gas volume at STP}} \times 1000$$

$$= \frac{6.33\ \text{mg}}{350\ \text{litres}} \times 1000$$

$$= 18.1\ \text{mg/m}^3$$

Note: multiply by 1000 to convert from litres to m^3 , as $1m^3$ = 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^2
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

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

$$= \frac{730\ \mu g}{8.5\ \text{litres}}$$

$$= 85.9\ \mu g/l\ \ (85.9\ mg/m^3)$$

8.2 Calculate the concentration of the substance at stack gas conditions

Stack temperature is 62 ^{o}C	Dry gas meter temperature is 10 ^{o}C (273K)
Stack pressure is 101.3 kPa	Reference pressure is 101.3 kPa
Stack moisture is 7%	Reference moisture is dry

Temperature correction factor

$$= \frac{\text{standard temperature}}{\text{stack temperature}}$$

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

$$= 0.815$$

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

= Concentration as measured x correction factor for temperature x correction factor for moisture

= 85.9 mg/m^3 x 0.815 x 0.93

= 65.1 mg/m^3

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^2
Seconds in 1 hour = 3600

Volume flow rate in m^3/s = average gas velocity in m/s x stack cross section area

= 10.4 m/s x 1.1 m^2

= 11.44 m^3/s

Volume flow rate in m^3/h = volume flow rate in m^3/s x seconds in 1 hour

= 11.4 m^3/s x 3600

= 41184 m^3/hr

8.4 Calculate the mass emission to atmosphere in g/hr

Mass emission rate = $\frac{\text{volume flow rate in the stack x concentration of substance}}{1000}$

= 41184 m^3/hr x 65.1 mg/m^3

= $\frac{\text{2681078 mg/hr}}{1000}$

= 2681 g/hr

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^3 (17 μg/l)

Detection limit = 1.3 μg/l

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

Mass of substance required in sample = 50 x LOD

= 50 x 1.3 μg/l

= 65 μg

Sample volume required $= \frac{\text{mass of substance required in sample}}{\text{concentration of substance in the stack}}$

$= \frac{65\ \mu g}{17\ \mu g/l}$

= 3.8 litres

Minimum sampling time required $= \frac{\text{sample volume required}}{\text{sampling rate}}$

$= \frac{3.8\ \text{litres}}{0.4\ \text{l/min}}$

= 9.5 minutes

10) To calculate the limit of detection expressed in terms of the concentration of the substance in the stack

Actual sampling time = 15 minutes
Sampling rate = 0.4 l/min

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

Detection limit = 1 µg

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

= 15 minutes x 0.4 l/min

= 6 litres

Mass of substance collected

= concentration of substance in the stack x sampled volume

= 17 µg/l x 6 litres

= 102 µg

Mass of substance collected as a multiple of the LOD

$$= \frac{\text{mass of substance collected}}{\text{LOD}}$$

$$= \frac{102\ \mu g}{1\ \mu g}$$

= 102

Relative limit of detection expressed in terms of the concentration of the substance in the stack

$$= \frac{\text{concentration of substance in the stack}}{\text{substance as a multiple of the LOD}}$$

$$= \frac{17\ \mu g/l}{102}$$

= 0.17 µg/l (0.17 mg/m^3)