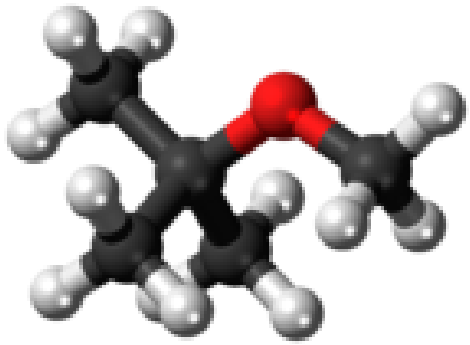
The Further Mathematics Support Programme

Balancing Chemical Equations



Methyl tert-butyl (MTBE) is an organic compound with molecular formula $(CH_3)_3COCH_3$.

MTBE is a flammable liquid that is used as a fuel additive, to raise the octane number and in place of Tetraethyl Lead to prevent 'knocking'.

In complete combustion it reacts with Oxygen to produce Carbon Dioxide and Water.

Suppose we wish to work out the chemical equation for this combustion.

We can simplify its molecular formula to $C_5H_{12}O$, so we have:

$$C_5H_{12}O + O_2 \rightarrow C0_2 + H_20$$

But the proportions of atoms on each side of the equation are not in balance and we need to work out the relative proportions of each molecule.

So let us assume that:

$$\mathbf{X_1}\, C_5H_{12}O + \mathbf{X_2}\, O_2 \rightarrow \mathbf{X_3}\, C0_2 + \mathbf{X_4}\, H_20$$

To make the calculation easier and as these are relative proportions, we can let $\mathbf{X_4} = 1$

Then:

$$\mathbf{X_1}\, C_5H_{12}O + \mathbf{X_2}\, O_2 \rightarrow \mathbf{X_3}\, C0_2 + H_20$$

Consider the number of carbon atoms on each side of the equation:

$5\, \mathbf{X_1} = \mathbf{X_3}$

Consider the number of hydrogen atoms on each side of the equation:

$12X_1 = 2$

Consider the number of oxygen atoms on each side of the equation:

$X_1 + 2X_2 = 2X_3 + 1$

These 3 equations can be solved relatively easily as fortunately one of the equations only contains one of the unknowns, but we will look at a more general method that will allow us to solve this system of equations, when each of the unknowns appears in every equation. Indeed the method can be generalised for any number of elements (not just three as in this case).

Rewriting the equations we have:

$5X_1 + 0X_2 - X_3 = 0$

$12X_1 + 0X_2 + 0X_3 = 2$

$X_1 + 2X_2 - 2X_3 = 1$

This can be written as a matrix equation:

$$\begin{pmatrix} 5 & 0 & -1 \\ 12 & 0 & 0 \\ 1 & 2 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix}$$

If we let $\mathbf{A} = \begin{pmatrix} 5 & 0 & -1 \\ 12 & 0 & 0 \\ 1 & 2 & -2 \end{pmatrix}$ then we have $\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \mathbf{A}^{-1} \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix}$

Where $\mathbf{A}^{-1}$ is the inverse of $\mathbf{A}$

Finding the inverse is a bit laborious but fortunately many calculators will do the job for us, so we can work out that:

$$\mathbf{A}^{-1} = \begin{pmatrix} 0 & \frac{1}{12} & 0 \\ -1 & \frac{3}{8} & \frac{1}{2} \\ -1 & \frac{5}{12} & 0 \end{pmatrix}$$

Hence using matrix multiplication we have $\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{12} & 0 \\ -1 & \frac{3}{8} & \frac{1}{2} \\ -1 & \frac{5}{12} & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{2}{12} \\ \frac{15}{12} \\ \frac{10}{12} \end{pmatrix}$

This means that $X_1 = \frac{2}{12}$ $X_2 = \frac{15}{12}$ $X_3 = \frac{10}{12}$

So multiplying through by 12 the proportions are 2, 15, 10 and 12

2 $C_5H_{12}O$ + **15** O_2 → **10** $C0_2$ + **12** H_20 is the balanced equation.

As a further example, consider the reaction of Sulphur with Nitric Acid:

$S + H_2NO_3 \rightarrow H_2SO_4 + NO_2 + H_2O$

Here we have 4 elements, so the required matrix will be 4 by 4. Considering the elements in the order in which they appear we have:

$\begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & 1 & 0 & -1 \\ 0 & 3 & -4 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \\ 0 \\ 1 \end{pmatrix}$ and this can be solved by finding the inverse of the 4 by 4 matrix, which is left as an exercise for the reader!

References

http://www.mathcentre.ac.uk/ [Accessed: 19/5/15] - an online drop-in centre for mathematics resources run by the Sigma Centre at Coventry University

http://ncalculators.com/matrix/ [Accessed: 19/5/15] – a set of matrix calculators

http://www.webqc.org/chemicaltools.php [Accessed: 19/5/15] – a website that has different calculators that are useful in Chemistry

http://en.wikipedia.org/wiki/Methyl_tert-butyl_ether [Accessed: 19/5/15] - Wikipedia information on MTBE