Gaussian Elimination and Chemical Equations [Andy Chong Sam]

Gaussian Elimination, a foundational technique of Linear Algebra, can be used to systematically balance chemical equations. Suppose we want to balance the following:

$$C_6H_{12}O_6 + O_2 \longrightarrow CO_2 + H_2O$$

The goal is to find coefficients a, b, c, and d such that:

$$\mathbf{a}\ C_6H_{12}O_6 + \mathbf{b}\ O_2 \longrightarrow \mathbf{c}\ CO_2 + \mathbf{d}\ H_2O$$

We start out by defining a vector that holds the number of atoms for each element on a given term. If we pick <C,H,O> the vector corresponding to the first term would be $< 6, 12, 6 >$. With this in mind, the problem can be reformulated:

$$a\begin{pmatrix}6\\12\\6\end{pmatrix} + b\begin{pmatrix}0\\0\\2\end{pmatrix} + c\begin{pmatrix}1\\0\\2\end{pmatrix} + d\begin{pmatrix}0\\2\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix} \quad \text{...In matrix form:} \quad \begin{pmatrix}6 & 0 & 1 & 0\\12 & 0 & 0 & 2\\6 & 2 & 2 & 1\end{pmatrix}$$

Elementary row operations are applied to simplify the system:

$$\begin{pmatrix}6 & 0 & 1 & 0\\12 & 0 & 0 & 2\\6 & 2 & 2 & 1\end{pmatrix} \xrightarrow{R_3 - R_1 = R_3} \begin{pmatrix}6 & 0 & 1 & 0\\12 & 0 & 0 & 2\\0 & 2 & 1 & 1\end{pmatrix}$$

For readability you can further apply operations to change the matrix to row echelon form but it's not entirely necessary. We can draw conclusions when no further cells can be canceled:

Since row 1 is $6a + c = 0$, let $a = 1$ and $c = -6$
Since row 2 is $12a + 2d = 0$, because a is 1, $d = -6$
Since row 3 is $2b + c + d = 0$, because $c = -6$, $d = -6$, then $b = 6$

If a coefficient is negative it just means it goes on the right side of the equation. The balanced equation is therefore:

$$C_6H_{12}O_6 + 6\,O_2 \longrightarrow 6\,CO_2 + 6\,H_2O$$

Also, we know the coefficients are correct since:

$$1\begin{pmatrix}6\\12\\6\end{pmatrix} + 6\begin{pmatrix}0\\0\\2\end{pmatrix} + -6\begin{pmatrix}1\\0\\2\end{pmatrix} + -6\begin{pmatrix}0\\2\\1\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix}$$

Two additional examples are provided on the next page.

Balance $\mathrm{As} + \mathrm{NaOH} \longrightarrow \mathrm{Na_3AsO_3} + \mathrm{H_2}$

The vector will be <As, Na, O, H> which produces the following system:

$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 3 & 0 \\ 0 & 1 & 3 & 0 \\ 0 & 1 & 0 & 2 \end{pmatrix}$$

A single row operation can be applied:

$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 3 & 0 \\ 0 & 1 & 3 & 0 \\ 0 & 1 & 0 & 2 \end{pmatrix} \xrightarrow{R_2 - R_3 = R_2} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 3 & 0 \\ 0 & 1 & 0 & 2 \end{pmatrix}$$

Row 1 gives us $a + c = 0$, let $a = 1$ and $c = -1$.
Row 3 gives us $b + 3c = 0$, since $c = -1$, $b = 3$.
Row 4 gives us $b + 2d = 0$, since $b = 3$, $d = -\frac{3}{2}$

Now this gives us $\mathrm{As} + 3\,\mathrm{NaOH} \longrightarrow \mathrm{Na_3AsO_3} + \frac{3}{2}\mathrm{H_2}$. We can't have partial coefficients so we'll multiply both sides by 2 to arrive at the solution:

$$2\,\mathrm{As} + 6\,\mathrm{NaOH} \longrightarrow 2\,\mathrm{Na_3AsO_3} + 3\,\mathrm{H_2}$$

Balance $\mathrm{NaOH} + \mathrm{H_2SO_4} \longrightarrow \mathrm{Na_2SO_4} + \mathrm{H_2O}$

The vector will be <Na, O, H, S>, so:

$$\begin{pmatrix} 1 & 0 & 2 & 0 \\ 1 & 4 & 4 & 1 \\ 1 & 2 & 0 & 2 \\ 0 & 1 & 1 & 0 \end{pmatrix} \xrightarrow{R_2 - 4R_4 = R_2} \begin{pmatrix} 1 & 0 & 2 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 2 & 0 & 2 \\ 0 & 1 & 1 & 0 \end{pmatrix} \xrightarrow{R_3 - R_2 = R_3} \begin{pmatrix} 1 & 0 & 2 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 2 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}$$

Row 1 is $a + 2c = 0$, let $a = 2$ so $c = -1$
Row 2 is $a + d = 0$, if $a = 2$ then $d = -2$
Row 3 is $2b + d = 0$, since $d = -2$ then $b = 1$
Row 4 is $b + c = 0$, if $b = 1$ then $c = -1$

We have the balanced equation:

$$2\,\mathrm{NaOH} + \mathrm{H_2SO_4} \longrightarrow \mathrm{Na_2SO_4} + 2\,\mathrm{H_2O}$$