Applications of Linear Algebra in Chemistry.

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Linear Algebra 2270-002

Linear Algebra extends its reaches into all parts of science and mathematics. In chemistry, one of linear algebras techniques (being the reduced row echelon form) can be used to solve one of chemistry's inescapable tasks of balancing chemical equations. Balancing chemical equations is fundamental when it comes to laboratory work as the correct ratios of reagents and products is vital to most chemical reactions. This task is taught and drilled into the head of students who study chemistry. The further a student studies chemistry the easier the task becomes but it can still be tedious and takes up valuable laboratory time. It can however be observed that when balancing a chemical equation, a system of equations can be formed from the process.

To make it simple let's start with a simple chemical reaction.

$$CH_4 + O_2 \rightarrow CO_2 + H_2O$$
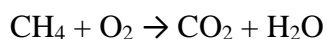
We are trying to determine the values of the coefficients in front of each compound so to start let's give each coefficient a letter value of X_1, X_2, X_3, X_4.

$$X_1\ CH_4 + X_2\ O_2 \rightarrow X_3\ CO_2 + X_4\ H_2O$$
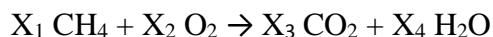
From looking at the equation, it can be seen that there are only three elements; Carbon, Hydrogen, and Oxygen, that make up the compounds in the equation. An equation can now be produced for each element by determining how many times that element shows up in the other compounds. For Carbon, one Carbon appears in X_1 and one appears in X_3 so the two can be set to each other resulting in the first equation $X_1 = X_3$. For Hydrogen, four appear in X_1 and two appear in X_4 so the corresponding equation is $4\ X_1 = 2\ X_4$. For Oxygen, there are two that appear in X_2, two in X_3, and one in X_4 so the following equation can be created $2\ X_2 = 2\ X_3 + X_4$. There are now three equations for each element and the system of equations can be formed:

$$\text{Carbon: } X_1 = X_3$$

$$\text{Hydrogen: } 4\ X_1 = 2\ X_4$$

$$\text{Oxygen: } 2\ X_2 = 2\ X_3 + X_4$$

This system of equations can be rewritten in standard form.

$$X_1 - X_3 = 0$$

$$4\,X_1 - 2\,X_4 = 0$$

$$2\,X_2 - 2\,X_3 - X_4 = 0$$

It can now be seen that these values can be placed into a matrix. From linear algebra we have learned that it is possible to reduce a matrix to produce specific values for a given variable in the equation set. The simplest method for doing so is by using the reduced row echelon form technique to solve for the value of the coefficients.

$$\begin{bmatrix} 1 & 0 & -1 & 0 & 0 \\ 4 & 0 & 0 & -2 & 0 \\ 0 & 2 & -2 & -1 & 0 \end{bmatrix} \approx \begin{bmatrix} 1 & 0 & 0 & -1/2 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1/2 & 0 \end{bmatrix}$$

With the reduced row echelon form solved for it can be seen that X_4 is a free variable and the solutions can be written as:

$$X_1 = 1/2\ X_4$$

$$X_2 = X_4$$

$$X_3 = 1/2\ X_4$$

To obtain full integers (generally preferred for chemists when doing lab work) the least common denominator between the equations must be found which in this case it is simple with
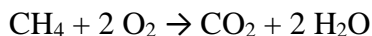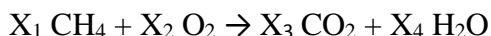
X_4 being equal to 2. This results in the final solution to the system of equations and these values can be placed into the original chemical equation.

$$X_1 = 1$$
$$X_2 = 2$$
$$X_3 = 1$$
$$X_4 = 2$$
$$X_1\ CH_4 + X_2\ O_2 \rightarrow X_3\ CO_2 + X_4\ H_2O$$

$$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$$

With the equation now balanced the method of utilizing a system of equations and solving for its reduced row echelon form proved to work. For this specific example, choosing an equation balancer is not necessary for the majority of chemists, since balancing it is simple and the method described above would most likely take most chemists longer to accomplish then to balance using traditional methods taught in the chemistry department. This method of balancing chemical equations however becomes useful when a chemical equation gets complex. For example:

$$MnS + As_2Cr_{10}O_{35} + H_2SO_4 \rightarrow HMnO_4 + AsH_3 + CrS_3O_{12} + H_2O$$

This example is used in Lay's book and slightly varies from the method described above for solving for the coefficients but it is essentially the same method to solve for the values. In this

equation however, instead of creating a system of equations by determining how many times each element appears in each compound, a vector is made for each compound. To help determine the values that will go into each matrix, a reference vector can be made for each compound.

$$\begin{bmatrix} Mn \\ S \\ As \\ Cr \\ O \\ H \end{bmatrix}$$

As done in the previous example each compound in the equation can be given a coefficient of X.

$$X_1 \; MnS + X_2 \; As_2Cr_{10}O_{35} + X_3 \; H_2SO_4 \rightarrow X_4 \; HMnO_4 + X_5 \; AsH_3 + X_6 \; CrS_3O_{12} + X_7 \; H_2O$$

Now for each coefficient value of X the values of how many times each element appears can be inputted into its respective matrix.

$$X_1\begin{bmatrix}1\\1\\0\\0\\0\\0\end{bmatrix}, X_2\begin{bmatrix}0\\0\\2\\10\\35\\0\end{bmatrix}, X_3\begin{bmatrix}0\\1\\0\\0\\4\\2\end{bmatrix} \rightarrow X_4\begin{bmatrix}1\\0\\0\\0\\4\\1\end{bmatrix}, X_5\begin{bmatrix}0\\0\\1\\0\\0\\3\end{bmatrix}, X_6\begin{bmatrix}0\\3\\0\\1\\12\\0\end{bmatrix}, X_7\begin{bmatrix}0\\0\\0\\0\\1\\2\end{bmatrix}$$

This set of vectors can be rewritten as the following:

$$X_1\begin{bmatrix}1\\1\\0\\0\\0\\0\end{bmatrix}+X_2\begin{bmatrix}0\\0\\2\\10\\35\\0\end{bmatrix}+X_3\begin{bmatrix}0\\1\\0\\0\\4\\2\end{bmatrix}+X_4\begin{bmatrix}-1\\0\\0\\0\\-4\\-1\end{bmatrix}+X_5\begin{bmatrix}0\\0\\-1\\0\\0\\-3\end{bmatrix}+X_6\begin{bmatrix}0\\-3\\0\\-1\\-12\\0\end{bmatrix}+X_7\begin{bmatrix}0\\0\\0\\0\\-1\\-2\end{bmatrix}=0$$

From this set of vectors, a matrix can be formed just as in the first example with the simple

chemical equation. From this matrix the reduced row echelon form can be found to determine the

values of the coefficients.

$$\begin{bmatrix}1 & 0 & 0 & -1 & 0 & 0 & 0\\1 & 0 & 1 & 0 & 0 & -3 & 0\\0 & 2 & 0 & 0 & -1 & 0 & 0\\0 & 10 & 0 & 0 & 0 & -1 & 0\\0 & 35 & 4 & -4 & 0 & -12 & -1\\0 & 0 & 2 & -1 & -3 & 0 & -2\end{bmatrix}\approx\begin{bmatrix}1 & 0 & 0 & 0 & 0 & 0 & -16/327\\0 & 1 & 0 & 0 & 0 & 0 & -13/327\\0 & 0 & 1 & 0 & 0 & 0 & -374/327\\0 & 0 & 0 & 1 & 0 & 0 & -16/327\\0 & 0 & 0 & 0 & 1 & 0 & -26/327\\0 & 0 & 0 & 0 & 0 & 1 & -130/327\end{bmatrix}$$

Now that the matrix has been reduced it is seen that X_7 is the free variable. The coefficients can

be written as:

$$X_1 = (16/327)\, X_7$$

$$X_2 = (13/327)\, X_7$$

$$X_3 = (374/327\, X_7$$

$$X_4 = (16/327)\, X_7$$

$$X_5 = (26/327)\, X_7$$

$$X_6 = (130/327)\, X_7$$

To obtain full integers as in the first example X_7 must be equal to 327 so the final balanced equation is:

$$16 \, MnS + 13 \, As_2Cr_{10}O_{35} + 374 \, H_2SO_4 \rightarrow 16 \, HMnO_4 + 26 \, AsH_3 + 130 \, CrS_3O_{12} + 327 \, H_2O$$

The following chemical equation would be difficult and tedious to balance by hand. In this case a linear algebra system would be of great use. Chemists in the field today are expected to have some form of coding experience. It wouldn't be too difficult a task for most to build a linear algebra system as described above but from personal lab experience most chemists will use online chemical equation balancers.

Chemical balance calculators are the easiest method to balance chemical equations because all that needs to be done is for the equation to be typed into the system and the system does the rest of the work. However, these systems are using the same linear algebra system of solving for the reduced row echelon form for a system of linear equations derived from a chemical equation. The easy part for chemists is that someone has already done all the work in building the linear algebra system. A commonly used online balancer is that of WolframAlpha. Based off my experience, most use this to quickly find the coefficients of the equation. Occasionally WolframAlpha will have hiccups on an equation so another common balancer is that of WebQC.

Citations

Lay, Steven R., David C. Lay, and Judi J. Mcdonald. *Linear Algebra and Its Applications (5th Edition)*. 5th ed. Pearson, 2015. Print.

"Equation Balancing." *Wolframalpha*. 2016. Web. 19 Apr. 2016. <https://www.wolframalpha.com/examples/ChemicalReactions.html>.

"Balance Chemical Equation." *WebQC*. 2016. Web. 19 Apr. 2016. <http://www.webqc.org/balance.php>.