# LINEAR ALGEBRA AND CHEMISTRY

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## 1. INTRODUCATION

Learning to take a matrix and put it in Reduced Row-Echelon Form takes a lot of time and practice but eventually, we learn how to do it. In any chemistry class, we must learn how to balance chemical reactions or equations, one of the foundations of chemistry. But looking at something like that for the first time can be really intimidating, I am going to explain why learning how to balance a chemical reaction is important and using linear algebra and the rules of Reduced Row-Echelon Form to make chemistry a little bit easier.

### BACKGROUND ON LINEAR ALGEBRA

One of the first things we learned in class was to take a system of linear equations and put it in reduced row-echelon form (RREF).

A matrix is in RREF when...

- any row with all zeros is at the bottom
- the first non-zero entry in a row is called the leading entry
- the leading entry is one row is to the right of the leading entry is any row above

Using (RREF) Gaussian (Gauss) Elimination, which consisted of

- scaling - multiplying by a non-zero number
- interchange - just switching the position of the equation
- replacement - multiplying one equation by a real number and adding it to another equation

It took a while to master but with practice, we can put any matrix in RREF and find the solutions. The same could be done with balancing chemical reactions in chemistry classes.

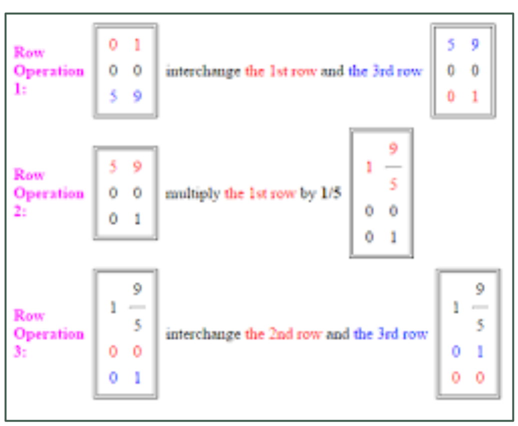


**Figure 1-1:Examples of scaling, interchange, and replacement and getting it to RREF**

## 2. BACKGROUND IN CHEMISTRY

Chemistry is the study of the composition, structure, and properties of matter. Using the periodic table, Figure 2-2, we can quickly reference information about elements like atomic mass and chemical symbols which we can see from Figure 2-1: because there is a lot of laboratory work in chemistry it is very important that you have this information available.

All chemical reactions have two parts...

1. The reactant is the substance you start with on the left side.
2. The product is the substance you end up with, the new substance that has been formed.

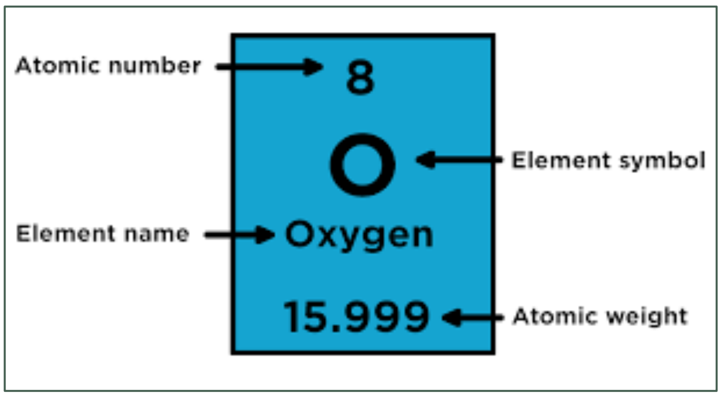


**Figure 2-1 This is an example of how you would see information about an element on the periodic table**

### LAW OF CONSERVATION OF MASS

"Every chemical reaction is the story of some chemical reaction."(Hamid, 521). In chemistry are laws that they must follow and one of them is called the law of conservation of mass, atoms cannot be created or destroyed which means that chemical equations must be balanced so what is on the right side must also be on the left side. A balanced equation has the same number of each element on both sides of the equation.

### BALANCING CHEMICAL REACTIONS AND WHY IS IT IMPORTANT?

To balance a chemical equation coefficient CAN be changed but subscripts CANNOT. To count atoms just multiply the coefficient and the subscript.

This is a systemic and formal way to solve chemical equations instead of guessing and checking your answer, "[which] can still be tedious and takes up valuable laboratory time"(Sanchez).

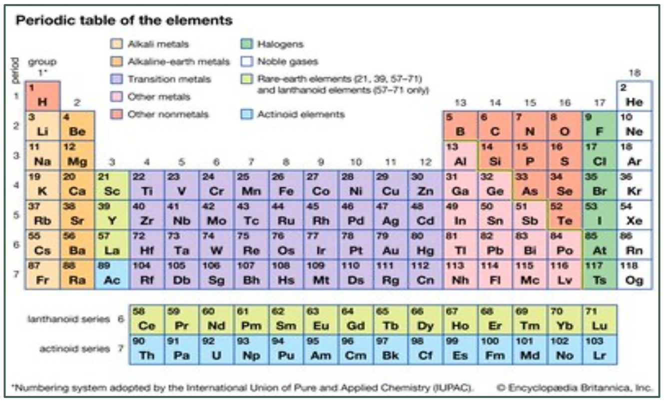


**Figure 2-2 Periodic Table**

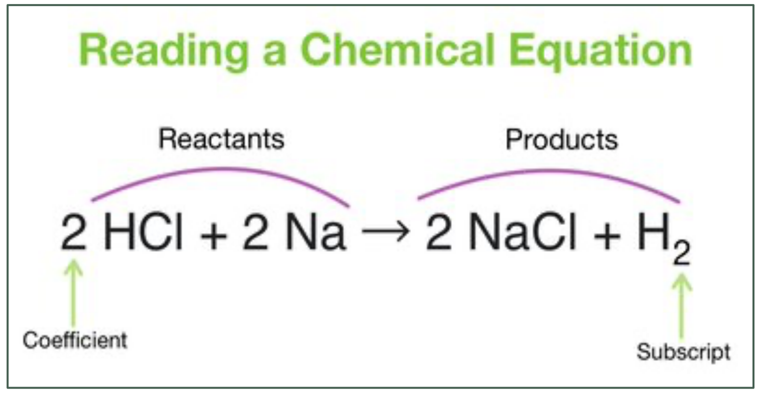


**Figure 2-3**

## 3. MATHEMATICAL IDEAS, COMPUTATION, AND EXAMPLES

*Balancing Chemical Equation by System of Linear Equations, by* Ihsanullah Hamid explains how we can use linear algebra without breaking the rules of chemistry, "The results satisfy the law of conservation... and confirm that there is no contradiction to the existing way(s) of balancing chemical equations"(Hamid 521). The author discusses that this approach can solve both "simple and advance chemical reactions typically encountered in the secondary chemistry classroom"(Hamid 521). Using Gauss Elimination, you can determine if the chemical reaction can be done, " A chemical reaction, when it is feasible, is a natural process, the consequent equation is always consistent. Therefore, we must have nontrivial solution. And we should be able to obtain its assuming existences. Such an assumption is absolutely valid and does not introduce any error. If the reaction is infeasible, then, there exists only a trivial solution, i.e., all coefficients are equal to zero"(Hamid 522).

This application is useful because it is neat and has a clear process even though each person might approach a matrix differently you will still end up with the identity matrix and the answers on the far right.

## EXAMPLE 1

$$C_2H_6 + O_2 \rightarrow CO_2 + H_2O \text{ -Not Balanced.}$$

The equation to balance is identified. This chemical reaction consists of three elements: Carbon(C); Hydrogen (H); Oxygen (O). The equation to balance is identified our task is to assign the unknowns coefficients $(x_1, x_2, x_3, x_4)$ to each chemical species. A balance equation can be written for each of these elements:

$$x_1C_2H_6 + x_2O_2 \rightarrow x_3CO_2 + x_4H_2O$$

Three simultaneous linear equations in four unknown corresponding to each of these elements. Then, the algebraic representation of the balanced

$$\text{Carbon}(C): 2x_1 = x_3 \Rightarrow 2x_1 - x_3 = 0$$

$$\text{Hydrogen}(H): 6x_1 = 2x_4 \Rightarrow 6x_1 - 2x_4 = 0$$

$$\text{Oxygen}(O): 2x_2 = 2x_3 + x_4 \Rightarrow 2x_2 - 2x_3 - x_4 = 0$$

First, note that there are four unknowns, but only three equations. The system is solved by Gauss elimination method as follows:

$$\left[\begin{array}{cccc|c} 2 & 0 & -1 & 0 & 0 \\ 6 & 0 & 0 & -2 & 0 \\ 0 & 2 & -2 & -1 & 0 \end{array}\right] \xrightarrow{R_2 \leftrightarrow R_2 - 3R_1} \left[\begin{array}{cccc|c} 2 & 0 & -1 & 0 & 0 \\ 0 & 0 & 3 & -2 & 0 \\ 0 & 2 & -2 & -1 & 0 \end{array}\right]$$

$$\xrightarrow{R_2 \leftrightarrow R_3} \left[\begin{array}{cccc|c} 2 & 0 & -1 & 0 & 0 \\ 0 & 2 & -2 & -1 & 0 \\ 0 & 0 & 3 & -2 & 0 \end{array}\right] \xrightarrow[R_1 \leftrightarrow 3R_1 + R_3]{R_2 \leftrightarrow 3R_2 + 2R_3} \left[\begin{array}{cccc|c} 6 & 0 & 0 & -2 & 0 \\ 0 & 6 & 0 & -7 & 0 \\ 0 & 0 & 3 & -2 & 0 \end{array}\right]$$

$$\xrightarrow{\substack{R_1 \leftrightarrow \frac{1}{6}R_1 \\ R_2 \leftrightarrow \frac{1}{6}R_2 \\ R_3 \leftrightarrow \frac{1}{3}R_3}} \left[\begin{array}{cccc|c} 1 & 0 & 0 & -1/3 & 0 \\ 0 & 1 & 0 & -7/6 & 0 \\ 0 & 0 & 1 & -2/3 & 0 \end{array}\right]$$

The last matrix is of reduced row echelon form, so we obtain that the solution of the system of linear equations is:

$$x_1 - \frac{1}{3}x_4 = 0 \Rightarrow x_1 = \frac{1}{3}x_4$$

$$x_2 - \frac{7}{6}x_4 = 0 \Rightarrow x_2 = \frac{7}{6}x_4$$

$$x_3 - \frac{2}{3}x_4 = 0 \Rightarrow x_3 = \frac{2}{3}x_4$$

where $x_4$ a free variable, particular solution is can then obtain by assigning values to the $x_4$, for instance $x_4 = 6$ we can represent the solution set as:

$$x_1 = 2,\ x_2 = 7,\ x_3 = 4$$

Thus, the balanced chemical reaction equation is:

$$2C_2H_6 + 7O_2 \rightarrow 4CO_2 + 6H_2O$$

**Figure 3-1 Shown is a chemical reaction with can be done using Gaussian Elimination**

As you can see from this example, we start out with a chemical equation and each coefficient is given a corresponding x-value.

Then we note the elements and how many of each element we have on both sides.

In the matrix, each element has its own row in the matrix as shown in Figure 3-1

1. Starts out with switching row 1 and row 2 with interchange then multiplying the new row 1 by -3 then adding it to row 2 as you can see that cancels out the 6.
2. Next row 3 and row 2 are interchanged because zeros belong on the bottom and there are 2 zeros in that row (replacement).
3. interchange row 2 and row 3 multiply 2 (row 3) and add it to row 3, then interchange row 1 and 3(row 1) and add it to row 3 (replacement)
4. Lastly, row 1 is scaled by 1/6, row 2 is scaled by 1/6, and row 3 1/3. As you can see the matrix is the identity matrix with the answers on the far right side.

### EXAMPLE 2

Consider this chemical reaction which is infeasible

$$K_4Fe(CN)_6 + K_2S_2O_3 \rightarrow CO_2 + K_2SO_4 + NO_2 + FeS \text{ -Not Balanced.}$$

A balance equation can be written for each of these elements:

$$x_1K_4Fe(CN)_6 + x_2K_2S_2O_3 \rightarrow x_3CO_2 + x_4K_2SO_4 + x_5NO_2 + x_6FeS$$

From above equation, we will obtain the following set of equations:

$$K: 4x_1 + 2x_2 = 2x_4$$
$$Fe: x_1 = x_6$$
$$C: 6x_1 = x_3$$
$$N: 6x_1 = 2x_5$$
$$S: 2x_2 = x_4 + x_6$$
$$O: 3x_2 = 2x_3 + 4x_4 + 2x_5$$

From the systems of equations we obtain the contradictions $x_2 = 3x_1$ and $x_2 = \frac{44}{3}x_1$, that means that the system is inconsistent, *i.e.*, we have only a trivial solution $x_i = 0(1 \le i \le 6)$. Hence, that means the chemical reaction is infeasible.

**Figure 3-2 Shown here is a chemical reaction which cannot be done because there are contradictions**

As you can see this chemical reaction cannot be done because there is a contradiction which is shown in Figure 3-2

## 4. CONCLUSION

As you can see from Figure 2.1, using linear algebra to solve chemical reactions/ equations is possible and you can tell from this method if the chemical reaction could occur. "Balancing chemical reaction is not chemistry, but it is just linear algebra. This study investigates that every chemical reaction is represented by homogenous systems of linear equations only" (Hamid 525). Which in turn can be put into a matrix and solved. I hope that this gives you some insight into how linear algebra can be applied in other studies like chemistry.

# CITATIONS


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