EN.535.441 Project Report: Application of Linear Systems

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1 Introduction

In this report we discuss the application of Gaussian elimination [1](which is a algorithm for solving a linear system of equations) to balance chemical equations as shown in [4].

2 Balancing chemical equations using Gaussian Elimination

According to law of conservation of matter [2] *In a chemical reaction, matter is neither created or destroyed.* So the number of atoms of a element on the reactant(left hand) side of the chemical equation should be equal to the number of atoms of a element on the product(right hand) side of the chemical equation.

$$\mathbf{2\,H_2 + O_2 \longrightarrow 2\,H_2O} \tag{1}$$

Therefore for each element in a unbalanced chemical equation we have a linear equation representing the relationship between the reactant and product sides. We can then use Gaussian elimination to solve these linear system of equations. We demonstrate this method by balancing the chemical equation for photosynthesis, oxidation of NADH.

2.1 Photosynthesis

The unnbalanced chemical equation for photosynthesis [3] is given by

$$\mathbf{xCO_2 + yH_2O \xrightarrow{sunlight} zO_2 + wC_6H_{12}O_6} \tag{2}$$

Writing the above in the form of linear equations

$$\begin{aligned} \mathbf{C} : x &= 6w \\ \mathbf{O} : 2x + y &= 2z + 6w \\ \mathbf{O} : 2y &= 12w \end{aligned}$$

Simplifying the above

$$\begin{aligned} x + 0y + 0z - 6w &= 0 \\ 2x + y - 2z - 6w &= 0 \\ 0x + 2y + 0z - 12w &= 0 \end{aligned}$$

Writing the equations in the augmented matrix form

$$\begin{bmatrix} 1 & 0 & 0 & -6 & 0 \\ 2 & 1 & -2 & -6 & 0 \\ 0 & 2 & 0 & -12 & 0 \end{bmatrix}$$

Applying the following row transformations to reduce the augmented matrix into row echelon form.

$$R_3 \to R_3/2$$

$$\begin{bmatrix} 1 & 0 & 0 & -6 & 0 \\ 2 & 1 & -2 & -6 & 0 \\ 0 & 1 & 0 & -6 & 0 \end{bmatrix}$$

$$R_2 \to R_2 - R_3$$

$$\begin{bmatrix} 1 & 0 & 0 & -6 & 0 \\ 2 & 0 & -2 & 0 & 0 \\ 0 & 1 & 0 & -6 & 0 \end{bmatrix}$$

$$R_2 \to R_2/2$$

$$\begin{bmatrix} 1 & 0 & 0 & -6 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & -6 & 0 \end{bmatrix}$$

$$R_1 \to R_1 - R_3$$

$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & -6 & 0 \end{bmatrix}$$

$$R_2 \to R_2 - R_1$$

$$\begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -6 & 0 \end{bmatrix}$$

From the above matrix we can write

$$\begin{aligned} x - y &= 0 \\ y - z &= 0 \\ y - 6w &= 0 \end{aligned}$$

The system has infinitely many solutions. Let w = 1, then we have y = 6, z = 6 and x = 6.

$$\mathbf{6\,CO_2 + 6\,H_2O \xrightarrow{sunlight} 6\,O_2 + C_6H_{12}O_6}$$

The equation (1) is now balanced.

2.2 Oxidation of NADH

The most important source of cellular energy is the synthesis of ATP (adenosine triphosphate) in our mitochondria. The synthesis of ATP is driven by the oxidation of NADH (nicotinamide adenine dinucleotide). The oxidation of NADH to NAD is catalyzed by NADH-CoQ reductase which removes 2 electrons from NADH to reduce Coenzyme Q. This electron transfer is coupled to the movement of protons across the membrane from the mitochondrial matrix to the intermembrane space. Its purpose is to create a proton gradient across the inner membrane called the proton-motive force. The ATP synthase uses the movement of protons down this gradient to power catalysis of ATP from ADP and phosphate. This process also requires the reduction of oxygen to water. How many molecules of oxygen do we need for every oxidized NADH?.

The unbalanced chemical equation is:

$$\mathbf{xNADH + yH + zO_2 \longrightarrow pNAD + qH_2O} \tag{3}$$

Writing the above in the form of linear equations

$$\mathbf{NAD}: x = p$$
$$\mathbf{H}: x + y = 2q$$
$$\mathbf{O}: 2z = q$$

Simplifying the above

$$x + 0y + 0z - p + 0q = 0$$
$$x + y + +0z + 0p - 2q = 0$$
$$0x + 0y + 2z + 0p - q = 0$$

Writing the equations in the augmented matrix form

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

Applying the following row transformations to reduce the augmented matrix into row echelon form.

$$R_2 \rightarrow R_2 - R_1$$
$$\begin{bmatrix} 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 1 & -2 & 0 \\ 0 & 0 & 2 & 0 & -1 & 0 \end{bmatrix}$$

From the above matrix we can write

$$x - p = 0$$
$$y + p - 2q = 0$$
$$2z - q = 0$$

The system has infinitely many solutions. Let p = 2, q = 2 then we have x = 2, z = 1 and y = 2.

$$\mathbf{2\,NADH + 2\,H + O_2 \longrightarrow 2\,NAD + 2\,H_2O}$$

The equation (3) is now balanced.

3 Conclusion

As shown with examples from photosynthesis and cellular respiration, Gaussian elimination can be used as a generic methodology to balance chemical equations. Converting the linear equations that relate the reactants and products into the augmented matrix form and, subsequently, row echelon form, to derive chemical coefficients is a much more straightforward method than the traditional trial-and-error process. Providing a more intuitive solution to this standard practice in chemistry can make the science more approachable and accessible to students being introduced to the material for the first time.

References

[1] http://mathworld.wolfram.com/GaussianElimination.html

[2] http://www.chemteam.info/Equations/Conserv-of-Mass.html

[3] https://msu.edu/user/morleyti/sun/Biology/photochem.html

[4] *Balancing Of Chemical Equations Using Matrix Algebra.* Cephas Iko-ojo Gabriel, Gerald Ikechukwu Onwuka