Application of the Concept of Linear Equation Systems in Balancing Chemical Reaction Equations

Dwindi Agryanti Johar[*]

Department of Mathematics, Universitas Padjadjaran, Sumedang, Indonesia

*Corresponding author email: dwindi19001@mail.unpad.ac.id

Abstract

This study discusses the equalization of chemical reactions using a system of linear equations with the Gaussian and Gauss-Jordan elimination. The results show that there is contradiction in the existing methods for balancing chemical reactions. This study also aims to criticize several studies that say that the equalization of the reaction coefficient can use a system of linear equations. In this paper, the chemical equations were balanced by representing the chemical equation into systems of linear equations. Particularly, the Gauss and Gauss-Jordan elimination methods were used to solve the mathematical problem with this method, it was possible to handle any chemical reaction with given reactants and products.

Keywords: balancing chemical reaction, linear equation, Gaussian Elimination, Gauss-Jordan Elimination, contradiction.

1. Introduction

Balancing of the chemical equation is one of the initial subjects taught in most preliminary chemistry courses (Hamid, 2019). A large number of research articles have been written on this topic for last two decades. It draws much attention of chemists who feel very difficult in the case of balancing typical chemical reaction equations (Hari Krishna et al., 2020). Balancing chemical reactions is an amazing subject matter for mathematics and chemistry students who want to see the power of linear algebra as a scientific discipline. Mass balance of chemical reactions is one of the most highly studied topics in chemical education (Risteski, 2012). This topic always draws the attention of students and teachers, but it is never a finished product. Because of its importance in chemistry and mathematics, there are several articles devoted to the subject. However, here we will not provide a historical perspective about this topic, because it has been done in so many previous publications (Risteski, 2014).

Algebra is a branch of science that discusses problems in the field of mathematics, one of which is the matrix. Matrix applications can be used to solve various kinds of solutions, for example in solving systems of linear equations, both systems of real linear equations and systems of complex linear equations (Aryani and Rizkiani, 2016). However, the system of linear equations that will be discussed in this study is a system of real linear equations. Several methods that are often used to solve systems of linear equations are the Gaussian and Gauss-Jordan elimination methods. Research on this method has been carried out, including research on (Baier et al., 2020; Ding and Schroeder, 2020; Schork and Gondzio, 2020; Pan and Zhao, 2017; Alonso et al., 2010; Geng et al., 2013). Then some research on Gauss-Jordan elimination can be seen in (David, 2016; Ma and Li, 2017; Anzt et al., 2018; Sheng, 2018), Based on the explanation and research, this paper focuses on balancing chemical reactions using a system of linear equations with the Cramer method and Gauss-Jordan elimination to see that a system of linear equations can be used to find the coefficient of each compound in chemical reaction equations.

2. Methodology

2.1. Linear Equation System

Definition of a linear equation: In general, a linear equation in n variable $x_1, x_2, ..., x_n$. can be expressed in terms of : $a_1x_1 + a_2x_2 + ... + a_nx_n = b$, where $a_1, a_2, ..., a_n$ and b are real constants. Variables in a linear equation are sometimes called independent variables.

  Definition of a system of linear equations: The finite set of linear equations - linear equations in n variable $x_1, x_2, ..., x_n$, is called a system of linear equations or a linear system. The general form of a system of linear equations which consists of m equations and n variable $x_1, x_2, ..., x_n$, can be written as

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + ... + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + ... + a_{2n}x_n &= b_n \\
&.. \\
a_{m1}x_1 + a_{m2}x_2 + ... + a_{mn}x_n &= b_m
\end{aligned}
\tag{1}
$$

Where a_{ij} and b_i $(1 \le i \le m, 1 \le j \le n)$ are Real constants. If viewed from the form of a system of linear equations in equation (1), it can also be expressed as

$$
\mathbf{AX = B}
\tag{2}
$$

$$
\text{With} \quad \mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & ... & a_{1n} \\ a_{21} & a_{22} & & a_{2n} \\ \vdots & & \ddots & \vdots \\ a_{m1} & a_{m2} & ... & a_{mn} \end{bmatrix}; \ \mathbf{X} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}; \ \mathbf{B} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}
\tag{3}
$$

Where A is the coefficient matrix of a system of linear equations.

  Adjustment of the Linear Equation System series of numbers $s_1, s_2, ..., s_n$ is called a solution to a system of linear equations if $x_1 = s_1, x_2 = s_2, ..., x_n = s_n$ is the solution of every equation in the system. A linear equation can have either a single (consistent) solution or an infinite (multiple solutions) and no (inconsistent) solution.

2.2 The Gaussian Elimination

Gaussian elimination method is based on method which applies various row operations in matrix in such manner which finally convert Augmented Matrix [A] in the form of upper triangular Matrix. Consider the system of linear equation

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + ... + a_{1n}x_n &= a_{1,n+1} \\
a_{21}x_1 + a_{22}x_2 + ... + a_{2n}x_n &= a_{2,n+1} \\
a_{31}x_1 + a_{32}x_2 + ... + a_{3n}x_n &= a_{3,n+1} \\
&... \\
a_{n1}x_1 + a_{n2}x_2 + ... + a_{nn}x_n &= a_{n,n+1}
\end{aligned}
\tag{4}
$$

This can be represented in matrix form as follows

$$
\begin{bmatrix} a_{11} & a_{12} & ... & a_{1n} \\ a_{21} & a_{22} & ... & a_{2n} \\ a_{31} & a_{32} & ... & a_{3n} \\ ... & ... & ... & ... \\ a_{n1} & a_{n2} & ... & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_{1,n+1} \\ a_{2,n+1} \\ a_{3,n+1} \\ ... \\ a_{n,n+1} \end{bmatrix}
\tag{5}
$$

  The algorithms consist of following three major steps

1. Read the Augment matrix A.
2. Reduce the matrix in upper triangular form.
3. Use backward substitution to get the solution.

If 0 is located on the diagonal, switch the rows until a nonzero is in that place. If shifting of row not possible then system has either infinite or no solution (Trivedi et al., 2017).

2.3 The Gauss-Jordan Elimination

In the Gauss elimination method, the coefficient matrix was reduced to an upper triangular matrix and the backward substitution was applied. **In Gauss-Jordan elimination method** the matrix is reduced into a diagonal matrix. At all steps of Gauss elimination method, the elimination is done not only for the lower diagonal entries but also the upper diagonal entries. Consider the system of linear equation

$$a_{11}x_1 + a_{12}x_2 + ... + a_{1n}x_n = a_{1,n+1}$$
$$a_{21}x_1 + a_{22}x_2 + ... + a_{2n}x_n = a_{2,n+1}$$
$$a_{31}x_1 + a_{32}x_2 + ... + a_{3n}x_n = a_{3,n+1} \tag{6}$$
$$...$$
$$a_{n1}x_1 + a_{n2}x_2 + ... + a_{nn}x_n = a_{n,n+1}$$

Where a_{ij} and $a_{i,j+1}$ are known constant and x_i are unknowns. The system is equivalent to $\mathbf{AX} = \mathbf{B}$. Where A is augmented matrix and X is column vector of unknown variable and B is Column Vector of Constant known as Constant vector. The general procedure for Gauss Jordan elimination can be summarized in the following steps.

1. Read the Augment matrix A.
2. Reduce the augmented matrix [A/b] to the transform A into diagonal form (pivoting).
3. Divide right-hand side's elements as well as diagonal elements by the diagonal elements in the row, which will make each diagonal element equal to one.

If 0 is located on the diagonal, switch the rows until a non-zero is in that place. If you are unable to do so, stop; the system has either infinite or no solution (Trivedi et al., 2017).

3. Results and Discussion

Problem 1.
Balance the following chemical reaction
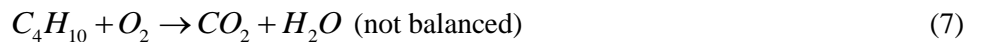
$$C_4H_{10} + O_2 \rightarrow CO_2 + H_2O \text{ (not balanced)} \tag{7}$$

Solution.
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:

$$x_1C_4H_{10} + x_2O_2 \rightarrow x_3CO_2 + x_4H_2O \tag{8}$$

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

$$\text{Carbon (C): } 4x_1 = x_3 \Rightarrow 4x_1 - x_3 = 0 \tag{9}$$
$$\text{Hydrogen (H): } 10x_1 = 2x_4 \Rightarrow 10x_1 - 2x_4 = 0 \tag{10}$$
$$\text{Oxygen (O): } 2x_2 = 2x_3 + x_4 \Rightarrow 2x_2 - 2x_3 - x_4 = 0 \tag{11}$$

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

$$\begin{bmatrix} 4 & 0 & -1 & 0 \\ 10 & 0 & 0 & -2 \\ 0 & 2 & -2 & -1 \end{bmatrix} : \begin{bmatrix} 1 & 0 & 0 & -0.2 \\ 0 & 1 & -1 & 0.5 \\ 0 & 0 & 1 & -0.8 \end{bmatrix}$$

Until this stage, the matrix is in Echelon-Row form, or by another name, it is called **Gaussian Elimination**. The next stage is

$$\begin{bmatrix} 1 & 0 & 0 & -0.2 \\ 0 & 1 & -1 & 0.5 \\ 0 & 0 & 1 & -0.8 \end{bmatrix} : \begin{bmatrix} 1 & 0 & 0 & -0.2 \\ 0 & 1 & 0 & -0.3 \\ 0 & 0 & 1 & -0.8 \end{bmatrix}$$

The matrix is now in a reduced line-echelon form, or by another name, it is called **Gauss-Jordan Elimination**. The last matrix is of reduced row echelon form, so we obtain that the solution of the system of linear equations is:

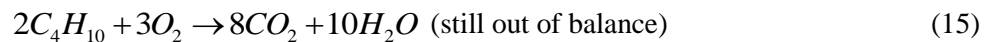$$x_1 - 0.2x_4 = 0 \rightarrow x_1 = 0.2x_4 \tag{12}$$
$$x_1 - 0.3x_4 = 0 \rightarrow x_1 = 0.3x_4 \tag{13}$$
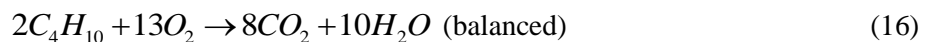$$x_3 - 0.8x_4 = 0 \rightarrow x_3 = 0.8x_4 \tag{14}$$

Where x_4 a free variable, particular solution is can then obtain by assigning values to the x_4 , for instance $x_4 = 10$ We can represent the solution set as:

$$x_1 = 2, x_2 = 3, x_3 = 8$$

The chemical reaction equation that we get based on the variables that we have been looking for is
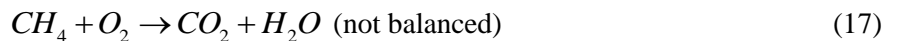
$$2C_4H_{10} + 3O_2 \rightarrow 8CO_2 + 10H_2O \text{ (still out of balance)} \tag{15}$$

The chemical equation that's supposed to be is

$$2C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O \text{ (balanced)} \tag{16}$$

Problem 2.
Balance the following chemical reaction

$$CH_4 + O_2 \rightarrow CO_2 + H_2O \text{ (not balanced)} \tag{17}$$

Solution.
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:

$$x_1CH_4 + x_2O_2 \rightarrow x_3CO_2 + x_4H_2O \tag{18}$$

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

$$\text{Carbon (C): } x_1 = x_3 \Rightarrow x_1 - x_3 = 0 \tag{19}$$
$$\text{Hydrogen (H): } 4x_1 = 2x_4 \Rightarrow 4x_1 - 2x_4 = 0 \tag{20}$$
$$\text{Oxygen (O): } 2x_2 = 2x_3 + x_4 \Rightarrow 2x_2 - 2x_3 - x_4 = 0 \tag{21}$$

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

$$\begin{bmatrix} 1 & 0 & -1 & 0 \\ 4 & 0 & 0 & -2 \\ 0 & 2 & -2 & -1 \end{bmatrix} : \begin{bmatrix} 1 & 0 & 0 & -0.5 \\ 0 & 1 & -1 & 0.5 \\ 0 & 0 & 1 & -0.5 \end{bmatrix}$$

Until this stage, the matrix is in Echelon-Row form, or by another name, it is called **Gaussian Elimination**. The next stage is

$$\begin{bmatrix} 1 & 0 & 0 & -0.5 \\ 0 & 1 & -1 & 0.5 \\ 0 & 0 & 1 & -0.5 \end{bmatrix} : \begin{bmatrix} 1 & 0 & 0 & -0.5 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -0.5 \end{bmatrix}$$

The matrix is now in a reduced line-echelon form, or by another name, it is called **Gauss-Jordan Elimination**. The last matrix is of reduced row echelon form, so we obtain that the solution of the system of linear equations is:

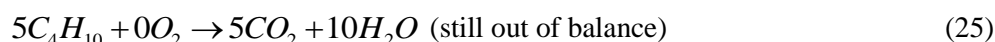$$x_1 - 0.5x_4 = 0 \rightarrow x_1 = 0.5x_4 \tag{22}$$
$$x_2 = 0 \tag{23}$$
$$x_3 - 0.5x_4 = 0 \rightarrow x_3 = 0.5x_4 \tag{24}$$

Where x_4 a free variable, particular solution is can then obtain by assigning values to the x_4, for instance $x_4 = 10$ We can represent the solution set as:

$$x_1 = 5, x_2 = 0, x_3 = 5$$

The chemical reaction equation that we get based on the variables that we have been looking for is

$$5C_4H_{10} + 0O_2 \rightarrow 5CO_2 + 10H_2O \text{ (still out of balance)} \tag{25}$$

The chemical equation that's supposed to be is

$$2C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O \text{ (balanced)} \tag{26}$$

4. Conclussion

From the research, it appears that the Gauss and Gauss-Jordan methods are not suitable to be applied to balancing chemical reactions. It sees from the calculation results that do not give results following the chemical reaction equivalence. This is in contradiction with previous studies that say that methods can be used. Suggestions for other researchers are to use another method or the same method is modified.

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