Linear systems on balancing chemical reaction problem

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Abstract. The concept of linear systems appears in a variety of applications. This paper presents a small sample of the wide variety of real-world problems regarding our study of linear systems. We show that the problem in balancing chemical reaction can be described by homogeneous linear systems. The solution of the systems is obtained by performing elementary row operations. The obtained solution represents the finding coefficients of chemical reaction. In addition, we present a computational calculation to show that mathematical software such as Matlab can be used to simplify completion of the systems, instead of manually using row operations.

1. Introduction
A chemical reaction is an expression showing a symbolic representation of the reactants and products [1]. The molecules to the left of the arrow are called reactants and those to the right the products. If the number of atoms for each type of element on the reactants is the same as the number of atoms of the corresponding type of the products, then the chemical reaction is said to be balanced [2], otherwise, it is not. The most important part of balancing chemical reaction is to determine the stoichiometric coefficients. There are two methods for balancing chemical reaction: by trial and algebraic [3]. The balancing by trial involves making successive intelligent guesses at making the coefficients that will balance a reaction equal and continue until the reaction attain the balance condition [4]. For simple chemical reactions, this method is very practical. However, for more complicated chemical reactions can take highly refined inspection. In this case, the algebraic is a systematic method that can overcome the looping provided in the trial method and can handle complex chemical reactions.

The algebraic method involves putting unknown coefficients in front of each molecule in the chemical reaction and solving for the unknown [3]. This then followed by write down the balance conditions on each element. There are various approaches that can be used. In this paper, we use systems of linear equations to balance chemical reaction. This proposed approach, we write down the systems in matrix form, obtain a homogeneous system of equations. We then perform elementary row operations on the matrix to obtain the solution of the systems. Furthermore, we present a computational calculation using Matlab to examine the obtained solution.

2. Methodology
2.1. Theoretical Basis
With referring to [2] we introduce the operation on the augmented matrix correspond to the equations in the associated system in order to solve the system. The operations below are called elementary row operations on a matrix:
1. Multiply a row through by a nonzero constant
2. Interchange two rows
3. Add constant time one row to another

Moreover, the augmented matrix can be simplified to a form from which the solution of the system can be ascertained by performing certain elementary row operations on the augmented matrix, by following below definition.

Definition 1. An $m \times n$ matrix $A$ is said to be in reduced row echelon form when the following properties are satisfied:
1. If a row does not consist entirely of zeros, then the first non-zero number in the row is a 1. We call this a leading 1.
2. If there are any rows that consist entirely of zeros, then they are grouped together at the bottom of the matrix.
3. In any two successive rows that do not consist entirely of zeros, the leading 1 in lower row occurs farther to the right than the leading 1 in the higher row.
   Each column that contains a leading 1 has zeros everywhere else in that column.

2.2. Numerical Examples
In this section, the use of linear systems to solve the problem of balancing chemical reaction is discussed. The objective is to find the stoichiometric coefficients that fulfill the reaction. All of the stoichiometric coefficients must be the smallest integer [5].

Example 1. Propane (C3H8) burns in oxygen to form carbon dioxide and steam (propane combustion reaction).

\[ \text{C3H8} + \text{O2} \rightarrow \text{CO2} + \text{H2O} \]

Let the stoichiometric coefficients be $a, b, c,$ and $d$ such that

\[ a\text{C3H8} + b\text{O2} \rightarrow c\text{CO2} + d\text{H2O} \]

We compare the number of Carbon (C), Hydrogen (H), and Oxygen (O) atoms of the reactants with the number of atoms of the products. We obtain the following set of equations in the table 1.

| Table 1. Stoichiometric coefficient. |
|--------------------------------------|
| **Left Side** | **Right Side** |
| Carbon         | $3a$         | $c$       |
| Hydrogen       | $8a$         | $2d$      |
| Oxygen         | $2b$         | $2c + d$  |

From which we obtain the homogeneous linear system

\[ \begin{bmatrix}
3 & 0 & -1 & 0 & a \\
8 & 0 & 0 & -2 & b \\
0 & 2 & -2 & -1 & c \\
0 & 0 & 0 & 0 & d
\end{bmatrix} = \begin{bmatrix}
0 \\
0 \\
0 \\
0
\end{bmatrix} \]

with augmented matrix for this system is

\[ \begin{bmatrix}
3 & 0 & -1 & 0 & 0 \\
8 & 0 & 0 & -2 & 0 \\
0 & 2 & -2 & -1 & 0
\end{bmatrix} \]

In the first step of elementary row operation, replace row two by three times row two minus eight times row one, i.e. $R_2 \leftrightarrow 3R_2 - 8R_1$ to yield
\[
\begin{bmatrix}
3 & 0 & -1 & 0 & 0 \\
0 & 0 & 8 & -6 & 0 \\
0 & 2 & -2 & -1 & 0
\end{bmatrix}
\]

Exchange a half row two with row three i.e. \( \frac{1}{2}R_2 \leftrightarrow R_3 \), yield
\[
\begin{bmatrix}
3 & 0 & -1 & 0 & 0 \\
0 & 2 & -2 & -1 & 0 \\
0 & 0 & 4 & -3 & 0
\end{bmatrix}
\]

Replace row one by four times row one plus row three \( R_1 \leftrightarrow 4R_1 + R_3 \) and replace row two by two times row two plus row three \( R_2 \leftrightarrow 2R_2 + R_3 \) to yield
\[
\begin{bmatrix}
12 & 0 & 0 & -3 & 0 \\
0 & 4 & 0 & -5 & 0 \\
0 & 0 & 4 & -3 & 0
\end{bmatrix}
\]

Replace row one with a twelfth-row one \( R_1 \leftrightarrow \frac{1}{12}R_1 \), row two with a fourth row two \( R_2 \leftrightarrow \frac{1}{4}R_2 \) and row three with a fourth row three \( R_3 \leftrightarrow \frac{1}{4}R_3 \) to obtain the reduced row echelon form
\[
\begin{bmatrix}
1 & 0 & 0 & -\frac{1}{4} & 0 \\
0 & 1 & 0 & -\frac{5}{4} & 0 \\
0 & 0 & 1 & -\frac{3}{4} & 0
\end{bmatrix}
\]

from which we conclude that the general solution of the system is
\[
\begin{align*}
\alpha &= \frac{1}{4}d, & \beta &= \frac{5}{4}d, & \gamma &= \frac{3}{4}d
\end{align*}
\]

where \( d \) is arbitrary. Let \( d = 4 \) so that \( \alpha = 1, \beta = 5 \) and \( \gamma = 3 \). Hence, the chemical reaction can be balanced as
\[
C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O
\]

**Example 2.** Consider the following reaction of sugar fermentation.
\[
C_6H_{12}O_6 \rightarrow CO_2 + C_2H_5OH
\]

Let \( a, b, \) and \( c \) be the stoichiometric coefficients such that
\[
aC_6H_{12}O_6 \rightarrow bCO_2 + cC_2H_5OH
\]

As in the previous example, for each of the atoms in the reaction, the number of atoms on the reactant must be equal to the number of atoms on the product. Then we obtain the following set of equations in the table 2.

| Table 2. Reaction of sugar fermentation. | Left Side | Right Side |
|----------------------------------------|-----------|------------|
| Carbon                                 | \( 6a \)  | \( b + 2c \) |
| Hydrogen                               | \( 12a \) | \( 6c \)    |
| Oxygen                                 | \( 6a \)  | \( 2b + c \) |

From which we obtain the homogeneous linear system
\[
\begin{bmatrix}
6 & -1 & -2 & a \\
12 & 0 & -6 & b \\
6 & -2 & -1 & c
\end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}
\]
with augmented matrix for this system is

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

The following elementary row operations \( R_2 \leftrightarrow R_2 - 2R_1 \) and \( R_3 \leftrightarrow R_3 - R_1 \) reduces the above matrix to

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

In the same vein, the following row operations \( R_2 \leftrightarrow \frac{1}{2}R_2 \) and \( R_3 \leftrightarrow 2R_3 + R_2 \) reduces the above matrix to

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

Finally, \( R_1 \leftrightarrow \frac{1}{6}R_1 + \frac{1}{6}R_2 \) reduces the matrix to the reduce row echelon form

\[
\begin{bmatrix}
1 & 0 & -\frac{1}{2} & 0 \\
0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 \\
\end{bmatrix}
\]

from which we conclude that the general solution of the system is

\[
a = \frac{1}{2}c, \quad b = c
\]

where \( c \) is arbitrary. Let \( c = 2 \) so that \( a = 1 \) and \( b = 2 \). Hence, the chemical reaction can be balanced as

\[
C_6H_{12}C_6 \rightarrow 2CO_2 + 2C_2H_5OH
\]

Example 3. Consider the following reaction of photosynthesis.

\[
CH_3COF + H_2O \rightarrow CH_3COOH + HF
\]

Let \( a, b, c \) and \( d \) be the stoichiometric coefficients such that

\[
aCH_3COF + bH_2O \rightarrow cCH_3COOH + dHF
\]

For each of the atoms in the reaction, the number of atoms on the reactant must be equal to the number of atoms on the product. Then we obtain the following set of equations in the table 3.

| Table 3. Reaction of photosynthesis. | Left Side | Right Side |
|-------------------------------------|-----------|------------|
| Carbon \( 2a \) | \( 2c \) |
| Hydrogen \( 3a + 2b \) | \( 4c + d \) |
| Oxygen \( a + b \) | \( 2c \) |
| Fluor \( a \) | \( d \) |

From which we obtain the homogeneous linear system

\[
\begin{bmatrix}
2 & 0 & -2 & 0 \\
3 & 2 & -4 & -1 \\
1 & 1 & -2 & 0 \\
1 & 0 & 0 & -1 \\
\end{bmatrix}
\begin{bmatrix}
a \\
b \\
c \\
d \\
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
\end{bmatrix}
\]

with augmented matrix for this system is
The following elementary row operations \( R_1 \leftrightarrow R_1 - 2R_4, \) \( R_2 \leftrightarrow R_2 - 3R_4 \) and \( R_3 \leftrightarrow R_3 - R_4 \) reduces the above matrix to

\[
\begin{bmatrix}
2 & 0 & -2 & 0 & 0 \\
3 & 2 & -4 & -1 & 0 \\
1 & 1 & -2 & 0 & 0 \\
1 & 0 & 0 & -1 & 0
\end{bmatrix}
\]

In the same vein, the following row operations \( -\frac{1}{2}R_1 \leftrightarrow R_4 \) and \( R_2 \leftrightarrow R_2 - 2R_3 \) reduces the above matrix to

\[
\begin{bmatrix}
1 & 0 & 0 & -1 & 0 \\
0 & 1 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & 0
\end{bmatrix}
\]

The following elementary row operations \( R_3 \leftrightarrow R_2 \) and \( R_3 \leftrightarrow R_3 + 2R_4 \) reduces the above matrix to

\[
\begin{bmatrix}
1 & 0 & 0 & -1 & 0 \\
0 & 1 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & 0
\end{bmatrix}
\]

Finally, \( R_4 \leftrightarrow R_3 \) reduces the matrix to the reduced row echelon form

\[
\begin{bmatrix}
1 & 0 & 0 & -1 & 0 \\
0 & 1 & 0 & -1 & 0 \\
0 & 0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

from which we conclude that the general solution of the system is

\[
a = d, \quad b = d, \quad c = d
\]

where \( d \) is arbitrary. Let \( d = 1 \) so that \( a = 1, b = 1 \) and \( c = 1 \). Hence, the chemical reaction can be balanced as

\[
\text{CH}_3\text{COF} + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{COOH} + \text{HF}
\]

2.3. Computational Results

In this section, we use Matlab to solve linear systems correspond to the chemical reactions given in the previous section. Remark that we constructed our Matlab program.

Example 4. Solving linear system given in example 1.

Type the augmented matrix \([3 \ 0 \ -1 \ 0 \ 0; \ 8 \ 0 \ -2 \ 0 \ 0; \ 0 \ 2 \ -2 \ -1 \ 0]\) on the terminal. If we run the program, then this gives the same reduced row echelon matrix as in example 1 (see figure 1).

![Figure 1. Reduced row echelon matrix on example 1 using Matlab.](image-url)
Hence, we obtain the solution as given in figure 2.

\[
\text{ans} = \\
\begin{bmatrix}
1 & 5 & 3 & 4
\end{bmatrix}
\]

**Figure 2.** The solution of the system of example 1 using Matlab.

Example 5. Solving linear system given in example 2.
Type the augmented matrix \[
\begin{bmatrix}
6 & -1 & -2 & 0; 12 & 0 & -6 & 0; 6 & -2 & -1 & 0
\end{bmatrix}
\] on the terminal. If we run the program, then this gives the same reduced row echelon matrix as in example 2 (see figure 3).

\[
\begin{bmatrix}
1.0000 & 0 & -0.5000 & 0 \\
0 & 1.0000 & -1.0000 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

**Figure 3.** The solution of the system of example 2 with Matlab.

Example 6. Solving linear system given in example 3.
Type the augmented matrix \[
\begin{bmatrix}
2 & 0 & -2 & 0 & 0; 3 & 2 & -4 & -1 & 0; 1 & 1 & -2 & 0 & 0; 1 & 0 & 0 & -1 & 0
\end{bmatrix}
\] on the terminal. If we run the program, then this gives the same reduced row echelon matrix as in example 3 (see figure 5).

\[
\begin{bmatrix}
1 & 0 & 0 & -1 & 0 \\
0 & 1 & 0 & -1 & 0 \\
0 & 0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

**Figure 4.** The solution of the system of example 3 using Matlab.

### 3. Conclusions
In this paper, we have shown how to balance chemical reactions using linear systems. In all the examples presented, the linear systems are suitable approach to balance chemical reactions problem. The elementary row operations that are applied to augmented matrix correspond to the equations in the associated system are easy to perform. The correctness of our manual calculation on each given examples have been confirmed by our Matlab program and it shows an excellent agreement.

### References
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