Balancing chemical equations using Gauss-Jordan Elimination aided by MATLAB

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Abstract- Balancing Chemical reaction equation (BCRE) is one of typical topic in Chemistry. The students are difficulty facing in balanced the chemical equation. Teachers find it difficult to teach while the students find it challenging to understand. Hence, this problem can be treated with solving a system of linear equation by transforming its augmented matrix of the corresponding system to reduced row echelon form using Gauss-Jordan elimination method aided by MATLAB.

Keywords – Augmented matrix, Chemical reaction, Gauss-Jordan elimination method, MATLAB

I. INTRODUCTION

Linear algebra is a cornerstone in undergraduate mathematical education. Here we are using one of the topic of linear algebra is Matrix algebra. BCRE is one of the important topic in chemistry, it becomes some cases difficulty, those cases BCRE by using Gauss-Jordan method. In chemical equation, the number of atoms for each element in the reaction and the total charge is the same for both the reactants and products are discussed by the following authors. Akinola *et.al* [1] studied row reduced echelon form in balancing a chemical equation. Nathan [2] discussed different tteaching mmethods for bbalancing chemical eequation. Smith *et.al* [3] explored an alternative method to Gauss-Jordan Elimination. Candelario [4] studied balancing chemical equations using Gauss-Jordan elimination aided by Matrix calculator. They have been many authors [5-15] studying BCRE by different principles in linear algebra for past years.

For chemists it is enough to find the minimal positive integer numbers of reactant and product must be equal during a chemical reaction. This study help chemistry students understand how to construct a homogenous system of linear equations whose solution provides suitable value to balance a chemical reaction equation using Gauss-Jordan elimination method.

II. FORMING HOMOGENENOUS LINEAR EQUATIONS

In this section principles in Linear Algebra (Matrix Algebra) are applied for balancing chemical reaction equations. The following chemical equations balancing techniques are so innovative that they will be more useful in balancing very difficult chemical reaction equations. There are a number of balancing techniques provided so far by researchers but the following method is completely differs from the previous methods. Besides the method discussed in this research article is very simple as per as previous methods considered. MATLAB Code is also presented here.

Prerequisites:

1) Every chemical reaction can be represented by the matrix equation $AX = O$ where A is called a reaction matrix and X is a column matrix of coefficients X_i and O is a null column matrix.

2) If the matrix equation $AX = 0$ has only trivial solution then corresponding chemical reaction is called infeasible reaction.

3) If the matrix equation $AX = 0$ has non trivial solution then corresponding chemical reaction is called feasible reaction.

Problem (1)

$$K_3[Fe(SCN)_6] + Na_2Cr_2O_7 + H_2SO_4 \rightarrow Fe(NO_3)_3 + Cr_2(SO_4)_3 + CO_2 + H_2O + Na_2SO_4 + KNO_3$$

The above chemical reaction equation is unbalanced. Where chemical elements are:
K-Potassium, Fe- Iron, S-Sulfur, C- Carbon, N- Nitrogen, Na-Sodium, Cr-Chromium, O-Oxygen, H-Hydrogen
Introducing unknowns $x_{i=1to9}$ in order to balance the above chemical equation,

$$x_1K_3[Fe(SCN)_6] + x_2Na_2Cr_2O_7 + x_3H_2SO_4 \rightarrow x_4Fe(NO_3)_3 + x_5Cr_2(SO_4)_3 + x_6CO_2 + x_7H_2O + x_8Na_2SO_4 + x_9\,KNO_3$$

Corresponding to eight elements one can get eight simultaneous linear equations as below these equations as a homogenous linear system in nine unknowns,

$$3x_1 - x_9 = 0$$
$$x_1 - x_4 = 0$$
$$6x_1 + x_3 - 3x_5 - x_8 = 0$$
$$6x_1 - x_6 = 0$$
$$6x_1 - 3x_4 + x_9 = 0$$
$$2x_2 - 2x_8 = 0$$
$$2x_2 - 2x_5 = 0$$
$$7x_2 + 4x_3 - 9x_4 - 12x_5 - 2x_6 - x_7 - 4x_8 - 3x_9$$
$$2x_3 - 2x_7 = 0$$

This system can be solved by Gauss-Jordan elimination method.
Consider the matrix equation AX=O

$$\text{Where } A = \begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 6 & 0 & 1 & 0 & -3 & 0 & 0 & -1 & 0 \\ 6 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 6 & 0 & 0 & -3 & 0 & 0 & 0 & 0 & -1 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & 2 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\ 0 & 7 & 4 & -9 & -12 & -2 & -1 & -4 & -3 \\ 0 & 0 & 2 & 0 & 0 & 0 & -2 & 0 & 0 \end{bmatrix} X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \end{bmatrix} O = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

where A is called reaction matrix.
The augmented matrix is given by

$$[A:O]=\begin{bmatrix} 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 6 & 0 & 1 & 0 & -3 & 0 & 0 & -1 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & -3 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 \\ 0 & 2 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 7 & 4 & -9 & -12 & -2 & -1 & -4 & -3 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & -2 & 0 & 0 & 0 \end{bmatrix}$$

Solving Augmented Matrix using Gauss-Jordan Elimination method
By applying row transformations one can get the echelon form as below

$$[A:O]=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1/3 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -16/3 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -58/3 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1/3 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -16/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -58/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -16/3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Number of unknowns (n)=9
Rank= number of non-zero rows=8

AX=O is a homogeneous linear system of equations and can have nontrivial solution as n>r i.e number of unknowns > rank.

Then System AX=O possess an infinitely many solutions. There are(n-r) number of linearly independent solutions.

Number of independent solutions is n–r=9-8=1

One can treat any one of $x_{i=1\,to\,9}$ as independent.

Let x_9 be independent. Then $x_1, x_2, \ldots x_8$ are dependent variables

For instance if one can choose

$$if\ x_9 = 3\ then\ we\ get\ x_1 = 1,\ x_2 = 16,\ x_3 = 58,\ x_4 = 1,\ x_5 = 16,\ x_6 = 6,\ x_7 = 58,\ x_8 = 16,$$

Since we have got a non-zero solution (non-trivial solution) the above chemical reaction equation in problem (1), therefore it is called feasible reaction equation.

Now the given chemical equation becomes

$$K_3[Fe(SCN)_6] + \mathbf{16}Na_2Cr_2O_7 + \mathbf{58}H_2SO_4 \rightarrow Fe(NO_3)_3 + \mathbf{16}Cr_2(SO_4)_3 + \mathbf{6}CO_2 + \mathbf{58}H_2O + \mathbf{16}Na_2SO_4 + \mathbf{3}\,KNO_3$$

Corresponding solution using MATLAB code

```
>> A =        [4 1 0 -1 0 0 0 0 0;
                1 0  0 0 -2 0 0 0 0;
                6 0  0 0 0 0 0 -1 0 ;
               6 0  0 0 0 0 -1 0 0;
```

```
0 1  0 0 0 -1 0 0 0;
0 4 4 -4 -12 -4 -3 -2 -1;
0 0 2 -1 0 0 -1 0 -2;
0 0 1 -1 -3 -1 0 0 0];
>>R = rref (A);
>>[N,D] = rat(R);
>>N;
>>D;
>>format rat
R
```

Problem (2).

Consider the following unbalanced chemical reaction

$$H_3PO_4 + (NH_4)_2MoO_4 + HNO_3 \rightarrow (NH_4)_3PO_4 * 12MoO_3 + NH_4NO_3 + H_2O$$

Say $y_1 H_3PO_4 + y_2\ (NH_4)_2MoO_4 + y_3\ HNO_3 \rightarrow y_4 (NH_4)_3PO_4.12MoO_3 + y_5\ NH_4NO_3 + y_6 H_2O$

It is unbalanced chemical equation and in this reaction there are five compounds

H- Hydrogen**;P-** Phosphorus**;O-** Oxygen**;N-** Nitrogen**;Mo-** Molybdenum

Introducing unknowns $x_{i=1\,to\,6}$ in order to balance the above chemical equation:

In the above equations subscript represents the total number of atoms of an element. Rewriting these equations as a homogenous linear system in four unknowns,

$$H: 3y_1 + 8y_2 + y_3 - 12y_4 - 4y_5 - 2y_6 = 0$$

$$P: y_1 - y_4 = 0$$

$$O: 4y_1 + 4y_2 + 3y_3 - 40y_4 - 3y_5 - y_6 = 0$$

$$N: 2y_2 + y_3 - 3y_4 - 2y_5 = 0$$

$$Mo: y_2 - 12y_4 = 0$$

This system can be solved by Gauss-Jordan elimination method.

Consider the matrix equation AX=O

$$\text{where} \quad A = \begin{bmatrix} 3 & 8 & 1 & -12 & -4 & -2 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 4 & 4 & 3 & -40 & -3 & -1 \\ 0 & 2 & 1 & -3 & -2 & 0 \\ 0 & 1 & 0 & -12 & 0 & 0 \end{bmatrix} \qquad X = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{bmatrix}, \ O = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The augmented matrix is given by

$$[A:O] = \begin{bmatrix} 3 & 8 & 1 & -12 & -4 & -2 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 4 & 4 & 3 & -40 & -3 & -1 & 0 \\ 0 & 2 & 1 & -3 & -2 & 0 & 0 \\ 0 & 1 & 0 & -12 & 0 & 0 & 0 \end{bmatrix}$$

Solving Augmented Matrix using Gauss-Jordan Elimination method

By applying row transformations one can get the Echelon form as below

$$[A:O]=\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & -1/12 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -7/4 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1/12 & 0 \\ 0 & 0 & 0 & 0 & 1 & -7/4 & 0 \end{bmatrix}$$

Treat y_6 as independent variable and remaining as dependent variables.

$$if\ \ y_6 = 12\ then\ y_1 = 1, y_2 = 12, y_3 = 21, y_4 = 1, y_5 = 21$$

Since we have got a non-zero solution (non-trivial solution) the above chemical reaction equation in problem (2), therefore it is called feasible reaction equation.

$$\mathrm{H_3PO_4} + \mathbf{12}\,\mathrm{(NH_4)_2MoO_4} + \mathbf{21}\,\mathrm{HNO_3} \rightarrow \mathrm{(NH_4)_3PO_4.12MoO_3} + \mathbf{21}\,\mathrm{NH_4NO_3} + \mathbf{12}\mathrm{H_2O}$$

Now the given chemical equation becomes

Corresponding solution using MATLAB code:

```
>> A=[ 3 8 1 -12 -4 -2;
        1 0 0 -1 0 0;
        4 4 3 -40 -3 -1;
   0 2 1 -3 -2 0;
   0 1 0 -12 0 0];
>>RR = rref (A);
>>[N,D] = rat(R);
>>N;
>>D;
>>format rat
R
```

III.CONCLUSION

Based on the results, BCRE can be taught and learned through the method of solving homogeneous linear equations by Gauss-Jordan elimination method. The utilization of MATLAB code may help the teachers in facilitating the learning of the topic. This software may also provide opportunities for the students to experience success, thus avoiding error and gaining interest in BCRE topic and linear algebra. Further, the application of MATLAB to other disciplines may also be conducted.

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