Application Of Gauss-Jordan Elimination Method In Balancing Typical Chemical Equations

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Abstract: Balancing equations in chemical reactions is very basic and fundamental concept and in some cases it becomes more difficult so that a mathematical treatment is needed in order to make it easy. This research paper mainly focuses on an excellent application of Gauss-Jordan elimination method in balancing typical unbalanced chemical equations. In fact, inspection is often the quickest and easiest way to balance complex equation. Here we are going to use Gauss-Jordan elimination method to balance a complicated chemical reaction equation. This method can be applied to balance any arbitrary given difficult chemical reaction. Besides MATLAB program related to this discourse has been presented in this research article.

Index Terms: Chemical reaction, Simultaneous linear equations, Balancing chemical equation, Homogenous linear equations, , Augmented matrix..

1. INTRODUCTION

BALANCING equations in chemical reactions is very basic and fundamental concept and in some cases it becomes more difficult so that a mathematical treatment is needed in order to make it easy. 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. An innovative mathematical treatment can make this typical work as very simple. Willian C. Herndon (1) in his research article presented a listing of some papers on chemical equation balancing which is most useful to research in chemistry. In addition to that he proposed comparative methods in balancing chemical reaction equations. Arcesio Garcia (2) in his research paper presented a very simple method which can be useful to any type of reaction which don't need the knowledge of oxidation numbers theory. Ice B. Risteski (3) in research discussion applied a new singular matrix method in chemical equation balancing and used the theory of solving homogenous equations by Drazin pseudo matrix. Lawrence R Thorn (4) in his paper presented an innovative method which deals with balancing of all chemical reaction equations using theory of matrix linear algebra. There have been a large number of researchers (5)-(29) studying balancing the chemical reaction equations using principles in Linear Algebra for last hundred years.

2 FORMING HOMOGENOUS 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).

$$K_4Fe(CN)_6 + KMnO_4 + H_2SO_4 = KHSO_4 + Fe_2(SO_4)_3 + MnSO_4 + HNO_3 + CO_2 + H_2O$$

It is unbalanced chemical equation where there are eight compounds and elements are:

K-Potassium,
Fe-Iron,
C-Carbon,
N-Nitrogen,
Mn-Manganese,
O-Oxygen,
H-Hydrogen,
S-Sulphur.

Introducing unknowns $y_i(i=1,2,...9)$ in order to balance the above chemical equation:

$$\mathbf{y_1}K_4Fe(CN)_6 + \mathbf{y_2}KMnO_4 + \mathbf{y_3}H_2SO_4 = \mathbf{y_4}KHSO_4 + \mathbf{y_5}Fe_2(SO_4)_3 + \mathbf{y_6}MnSO_4 + \mathbf{y_7}HNO_3 + \mathbf{y_8}CO_2 + \mathbf{y_9}H_2O$$

Corresponding to eight elements one can get eight simultaneous linear equations as below

$K \quad 4y_1 + y_2 = y_4$

$Fe \quad y_1 = 2y_5$

$C \quad 6y_1 = y_8$

$N \quad 6y_1 = y_7$

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$Mn \quad y_2 = y_6$

$O \quad 4y_2 + 4y_3 = 4y_4 + 12y_5 + 4y_6 + 3y_7 + 2y_8 + y_9$

$H \quad 2y_3 = y_4 + y_7 + 2y_9$

$S \quad y_3 = y_4 + 3y_5 + y_6$

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

$$4y_1 + y_2 - y_4 = 0$$
$$y_1 - 2y_5 = 0$$
$$6y_1 - y_8 = 0$$
$$6y_1 - y_7 = 0$$
$$y_2 - y_6 = 0$$
$$4y_2 + 4y_3 - 4y_4 - 12y_5 - 4y_6 - 3y_7 - 2y_8 - y_9 = 0$$
$$2y_3 - y_4 - y_7 - 2y_9 = 0$$
$$y_3 - y_4 - 3y_5 - y_6 = 0$$

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

Consider the matrix equation AX=O

where
$$A = \begin{bmatrix} 4 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 6 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 4 & 4 & -4 & -12 & -4 & -3 & -2 & -1 \\ 0 & 0 & 2 & -1 & 0 & 0 & -1 & 0 & -2 \\ 0 & 0 & 1 & -1 & -3 & -1 & 0 & 0 & 0 \end{bmatrix}$$

$$X = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \end{bmatrix} \qquad O = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

where A is called reaction matrix.

The augmented matrix is given by

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

Solving Augmented Matrix using Gauss-Jordan Elimination method

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

$$[A \vdots O] = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -5/94 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -61/94 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -299/188 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -81/94 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -5/188 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -61/94 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -15/47 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -15/47 & 0 \end{bmatrix}$$

Number of unknowns (n)=9 $y_i (i = 1,2,..9)$

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.

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

One can treat any one of $y_i (i = 1,2,..9)$ as independent.

Let y_9 be independent.

Then $y_1, y_2, ...y_8$ are dependent variables

If n=r, then the system AX=O possess just trivial solution i.e zero solution only.

For the system AX=O:

n>r	System AX=O possess an infinitely many solutions. There are(n-r) number of linearly independent solutions.
n=r	System AX=O possess only one solution which is trivial solution or zero solution. Number of linearly independent solutions is zero.

For instance if one can choose

If $y_9 = 188$,

then we get $y_1 = 10, y_2 = 122$,

$y_3 = 299, y_4 = 162, y_5 = 5, y_6 = 122, y_7 = 60, y_8 = 60$

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

$$\mathbf{10}K_4Fe(CN)_6 + \mathbf{122}KMnO_4 + \mathbf{299}H_2SO_4 = \mathbf{162}KHSO_4 + \mathbf{5}Fe_2(SO_4)_3 + \mathbf{122}MnSO_4 + \mathbf{60}HNO_3 + \mathbf{60}CO_2 + \mathbf{188}H_2O$$

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

$$x_1FeCl_2 + x_2Na_3PO_4 = x_3Fe_3(PO_4)_2 + x_4NaCl$$

It is unbalanced chemical equation and in this reaction there are four compounds
Fe-Iron,
Cl-Chlorine,
Na-Sodium,
P-Phosphorus,
O-Oxygen.

Introducing unknowns $x_i (i = 1,2,3,4)$ in order to balance the above chemical equation:

$$x_1FeCl_2 + x_2Na_3PO_4 = x_3Fe_3(PO_4)_2 + x_4NaCl$$

Corresponding to five elements one can get five simultaneous linear equations as below

$$\begin{array}{ll} Fe & x_1 = 3x_3 \\ Cl & 2x_1 = x_4 \\ Na & 3x_2 = x_4 \\ P & x_2 = 2x_3 \\ O & 4x_2 = 8x_3 \end{array}$$

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,

$$\begin{array}{ll} Fe & x_1 - 3x_3 = 0 \\ Cl & 2x_1 - x_4 = 0 \\ Na & 3x_2 - x_4 = 0 \\ P & x_2 - 2x_3 = 0 \\ O & 4x_2 - 8x_3 = 0 \end{array}$$

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

where $$A = \begin{bmatrix} 1 & 0 & -3 & 0 \\ 2 & 0 & 0 & -1 \\ 0 & 3 & 0 & -1 \\ 0 & 1 & -2 & 0 \\ 0 & 4 & -8 & 0 \end{bmatrix} \quad X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \quad O = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The augmented matrix is given by

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

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

$$[A \vdots O] = \begin{bmatrix} 1 & 0 & 0 & -1/2 & 0 \\ 0 & 1 & 0 & -1/3 & 0 \\ 0 & 0 & 1 & -1/6 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Treat x_4 as independent variable and remaining as dependent variables.

If $x_4 = 6,$ then $x_1 = 3, x_2 = 2, x_3 = 1$

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.
Now the given chemical equation becomes

$$\mathbf{3}FeCl_2 + \mathbf{2}Na_3PO_4 = \mathbf{1}Fe_3(PO_4)_2 + \mathbf{6}NaCl$$

MATLAB code:

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

4 CONCLUSION

In the above research article a generalized method of balancing chemical reaction equations using the method of solving homogeneous linear equations by Gauss-Jordan elimination method has been proposed. Besides the relative MATLAB code is also given in the above paper. In the context of future research one can extend these ideas to develop a more general method which helps in deterring whether a complicated chemical reaction equations having any arbitrary number of compounds and elements is feasible or not.

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