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UE18MA251- LINEAR ALGEBRA

MINI PROJECT REPORT

ON

Balancing the Chemical Equation using reduced row echelon form

Submitted by

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Branch & Section : Computer Science 'A' Section

PROJECT EVALUATION

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Sl.No.	Parameter	Max Marks	Marks Awarded
1	Background & Framing of the problem	4	
2	Approach and Solution	4	
3	References	4	
4	Clarity of the concepts & Creativity	4	
5	Choice of examples and understanding of the topic	4	
6	Presentation of the work	5	
	Total	25	

Name of the Course Instructor :

Signature of the Course Instructor :

Introduction

Balancing of the chemical equation is one of the initial subjects taught in most preliminary chemistry courses. Balancing chemical reactions is an amazing subject of matter for mathematics and chemistry students who want to see the power of linear algebra as a scientific discipline. Since the balancing of chemical reactions in chemistry is a basic and fundamental issue, it deserves to be considered on a satisfactory level. A chemical equation is only a symbolic representation of a chemical reaction. Actually, every chemical equation is the story of some chemical reaction. Chemical equations play a main role in theoretical as well as in industrial chemistry. A chemical reaction can neither create nor destroy atoms. So, all of the atoms represented on the left side of the arrow must also be on the right side of the arrow. This is called balancing the chemical equation. The application of the law of conservation of matter is critical in chemistry education and is demonstrated in practice through balanced chemical equations. Every student who has general chemistry as a subject is bound to come across balancing chemical equations. The substances initially involved in a chemical reaction are called reactants, but the newly formed substances are called the products. The products are new substances with properties that are different from those of reactants. A chemical equation is said to be balanced, the number of atoms of each type on the left is the same as the number of atoms of corresponding type on the right.

Balancing chemical equation by inspection is often believed to be a trial and error process and, therefore, it can be used only for simple chemical reactions. But still it has limitations. Balancing by inspection does not produce a systematic evaluation of all of the sets of coefficients that would potentially balance an equation. Another common method of balancing chemical reaction equations is the algebraic approach. In this approach, coefficients are treated as unknown variables or undetermined coefficients whose values are found by solving a set of simultaneous equations. According to, the author clearly indicated that the algebraic approach to balancing both simple and advance chemical reactions typically encountered in the secondary chemistry classroom is superior to that of the inspection method. Also, in, the author emphasized very clearly that balancing chemical reactions is not chemistry; it is just linear algebra. From a scientific viewpoint, a chemical reaction can be balanced if only it generates a vector space. That is a necessary and sufficient condition for balancing a chemical reaction.

A chemical reaction, when it is feasible, is a natural process, the consequent equation is always consistent. Therefore, we must have nontrivial solution. And we should be able to obtain its assuming existences. Such an assumption is absolutely valid and does not introduce any error. If the reaction is infeasible, then, there exists only a trivial solution, i.e., all coefficients are equal to zero. In Mathematics and Chemistry, there are several mathematical methods for balancing chemical reactions. All of them are based on generalized matrix inverses and they have formal scientific properties that need a higher level of mathematical knowledge for their application. Here, we are presenting the Gauss elimination method, it was possible to handle any chemical reaction with given reactants and products. Solved problems are provided to show that this methodology lends well for both simple and complex reactions.

Methodology

In this section, we state well known results about echelon form and row reduced echelon form.

The number of nonzero rows and columns are the same in any echelon form produced from a given matrix A by elementary row operations, irrespective of the sequence of row operations used.

Given an n m× matrix A,

1. Use Gauss elimination to produce an echelon form from A.

2. Use the bottom-most non zero entry 1 in each leading column of the echelon form, starting with the rightmost leading column and working to the left, so as to eliminate all non-zero entries in that column strictly above that entry one.

Row-reduced echelon: An n m× matrix A is said to be in row reduced echelon from when:

1. It is in echelon form (with k non-zero rows, say)

2. The i the leading column equals i e , the i the column of the identity matrix of order p , for 1 ≤ ≤i k .

Stepwise Solution to Balance the Chemical Equation with an example:

1. Identify the equation to balance.

- $$H_3PO_4 + (NH_4)_2MoO_4 + HNO_3 \rightarrow (NH_4)_3PO_4 \cdot 12\,MoO_3 + NH_4NO_3 + H_2O$$

2. Identify the elements.

The number of elements present in the equation determines how many rows will be in the vectors and matrices that we are going to construct. Below, the order we list corresponds to the order of the rows.

- H – Hydrogen
- P – Phosphorus
- O – Oxygen
- N – Nitrogen
- Mo – Molybdenum

3. Set up the vector equation.

The vector equation consists of column vectors corresponding to each compound in the equation. Each vector has a corresponding coefficient, labeled to for which we are solving for. Make sure you understand how to count the number of atoms in a molecule.

- $x_1 \begin{pmatrix} 3 \\ 1 \\ 4 \\ 0 \\ 0 \end{pmatrix} + x_2 \begin{pmatrix} 8 \\ 0 \\ 4 \\ 2 \\ 1 \end{pmatrix} + x_3 \begin{pmatrix} 1 \\ 0 \\ 3 \\ 1 \\ 0 \end{pmatrix} = x_4 \begin{pmatrix} 12 \\ 1 \\ 40 \\ 3 \\ 12 \end{pmatrix} + x_5 \begin{pmatrix} 4 \\ 0 \\ 3 \\ 2 \\ 0 \end{pmatrix} + x_6 \begin{pmatrix} 2 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

4. Set the equation to 0 and obtain the augmented matrix.

There are two major points to consider here. First, recognize that a vector equation like the one above has the same solution set as a linear system with its corresponding augmented matrix. This is a fundamental idea in linear algebra. Second, when the augments are all 0, row-reduction does not change the augments. Therefore, we need not write them at all – row-reducing the coefficient matrix is all that is necessary.

Note that moving everything to the left side causes the elements on the right side to negate.

$$\begin{pmatrix} 3 & 8 & 1 & -12 & -4 & -2 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 4 & 4 & 3 & -40 & -3 & -1 \end{pmatrix}$$

5. Row-reduce to reduced row-echelon form.

For such a matrix, it is recommended that you use a calculator, although row-reducing by hand is always an option, albeit slower.

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & -1/12 \\ 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & -7/4 \\ 0 & 0 & 0 & 1 & 0 & -1/12 \\ 0 & 0 & 0 & 0 & 1 & -7/4 \end{pmatrix}$$

It is clear that there is a free variable here. Those with sharp minds would've seen this coming, for there are more variables than equations, and hence more columns than rows. This free variable means that can take on any value, and the resulting combination of to would be a valid solution (to our linear system, that is – the chemical equation results in further restrictions in this solution set).

6. Parameterize the free variable and solve for the variables.

Let's set Since for positive values of none of the variables become negative, so we are on the right track.

- $x_1 = t/12$
- $x_2 = t$
- $x_3 = 7t/4$
- $x_4 = t/12$
- $x_5 = 7t/4$
- $x_6 = t$

7. Substitute an appropriate value for t.

Remember that the coefficients in the chemical equation must be integers. Therefore, set t=12 the least common multiple. From our solution set, it is clear that while there are an infinite number of solutions, as we would expect, it is nonetheless a *countably* infinite set.

- $x_1 = 1$
- $x_2 = 12$
- $x_3 = 21$
- $x_4 = 1$
- $x_5 = 21$
- $x_6 = 12$

8. Substitute the coefficients into the chemical equation.
The equation is now balanced.

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

Worked Examples

1) Rust is formed when there is a chemical reaction between iron and oxygen. The compound that is formed is a reddish-brown scale that covers the iron object. Rust is an iron oxide whose chemical formula is Fe2O3, so the chemical formula for rust is

$$\mathrm{Fe} + \mathrm{O_2} \rightarrow \mathrm{Fe_2O_3}.$$

Balance the equation.

In balancing the equation, let p q, and r be the unknown variables such that

$$p\mathrm{Fe} + q\mathrm{O_2} \rightarrow r\mathrm{Fe_2O_3}.$$

We compare the number of Iron (Fe) and Oxygen (O) atoms of the reactants with the number of atoms of the product. We obtain the following set of equations:

$$\mathrm{Fe}: p = 2r$$
$$\mathrm{O}: 2q = 3r,$$

The homogeneous system of equations becomes

$$\begin{bmatrix} 1 & 0 & -2 \\ 0 & 2 & -3 \end{bmatrix} \begin{bmatrix} p \\ q \\ r \end{bmatrix} = \mathbf{0}, \quad \text{where} \quad \boldsymbol{A} = \begin{bmatrix} 1 & 0 & -2 \\ 0 & 2 & -3 \end{bmatrix}.$$

From the above, the matrix A is already in the echelon form U, with two pivots 1 and 2 but not in row reduced echelon form, even though there is a zero above the second pivot 2. However, to reduce it to row reduced echelon form R; all the pivots must be one. Hence, we replace row two with half row two, that is R2 <->R2 -2R1 to yield,

$$\boldsymbol{R} = \begin{bmatrix} 1 & 0 & -2 \\ 0 & 1 & -\frac{3}{2} \end{bmatrix}.$$

Thus, Rx = 0 becomes

$$\begin{bmatrix} 1 & 0 & -2 \\ 0 & 1 & -\frac{3}{2} \end{bmatrix} \begin{bmatrix} p \\ q \\ r \end{bmatrix} = \mathbf{0}.$$

Upon expanding, we have

$$p - 2r = 0 \quad \text{or} \quad p = 2r$$

$$q - \frac{3}{2}r = 0 \quad \text{or} \quad q = \frac{3}{2}r,$$

the null space solution

$$\boldsymbol{x} = \begin{bmatrix} p \\ q \\ r \end{bmatrix} = \begin{bmatrix} 2 \\ \frac{3}{2} \\ 1 \end{bmatrix} r.$$

There are three pivot variables p q, and one free variable r . If we choose r = 1 , then , p=2 q =3/2 . To avoid fractions, we can also let r = 2 , so that p q = = 4, 3 and r = 2 . We remark that these are not the only solutions since there is a free variable r , the null space solution is infinitely many. Therefore, the chemical equation can be balanced as

$$2\mathrm{Fe}+\frac{3}{2}\mathrm{O}_2 \to \mathrm{Fe}_2\mathrm{O}_3,$$

or

$$4\mathrm{Fe}+3\mathrm{O}_2 \to 2\mathrm{Fe}_2\mathrm{O}_3.$$

Example 2

Ethane (C2H6) burns in oxygen to produce carbon (IV) oxide CO2 and steam. The steam condenses to form droplets of water.

$$\mathrm{C}_2\mathrm{H}_6+\mathrm{O}_2 \to \mathrm{CO}_2+\mathrm{H}_2\mathrm{O},$$

Balance the equation. Let the unknowns be p, q, r and s such that,

$$p\mathrm{C}_2\mathrm{H}_6+q\mathrm{O}_2 \to r\mathrm{CO}_2+s\mathrm{H}_2\mathrm{O}.$$

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:

$$\begin{aligned} \mathrm{C}&: 2p = r \\ \mathrm{H}&: 6p = 2s \\ \mathrm{O}&: 2q = 2r + s. \end{aligned}$$

In homogeneous form,

$$\begin{bmatrix} 2 & 0 & -1 & 0 \\ 6 & 0 & 0 & -2 \\ 0 & 2 & -2 & -1 \end{bmatrix}\begin{bmatrix} p \\ q \\ r \\ s \end{bmatrix}=\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

In the first step of elimination, replace row two by row two minus three times row one, i.e., 2 21 R RR ↔ − 3 to yield,

$$\sim\begin{bmatrix} 2 & 0 & -1 & 0 \\ 0 & 0 & 3 & -2 \\ 0 & 2 & -2 & -1 \end{bmatrix}.$$

Exchange row two with row three or vice versa to reduce A to echelon form U ,

$$U = \begin{bmatrix} 2 & 0 & -1 & 0 \\ 0 & 2 & -2 & -1 \\ 0 & 0 & 3 & -2 \end{bmatrix}.$$

In the next set of operations that we will carry out to reduce U to R , we perform row operations that will change the entries above the pivots to zero; Replace row one by three times row two plus two times row three i.e. R2 ↔3R2+2R3 and replace row one with three times row one plus row three (R1↔3R1 +R3) to yield,

$$\begin{bmatrix} 6 & 0 & 0 & -2 \\ 0 & 6 & 0 & -7 \\ 0 & 0 & 3 & -2 \end{bmatrix}$$

The last operation that will give us R , is to reduce all the pivots to unity, that is replace row one with one-sixth row one, row two with one-sixth row two and row three with one-third row three to obtain

$$R = \begin{bmatrix} 1 & 0 & 0 & -\frac{1}{3} \\ 0 & 1 & 0 & -\frac{7}{6} \\ 0 & 0 & 1 & -\frac{2}{3} \end{bmatrix}.$$

The solution to Ax = 0 reduces to Rx = 0 where x is actually the null space of A which is equivalent to the null space of R. Hence,

$$\begin{bmatrix} 1 & 0 & 0 & -\frac{1}{3} \\ 0 & 1 & 0 & -\frac{7}{6} \\ 0 & 0 & 1 & -\frac{2}{3} \end{bmatrix} \begin{bmatrix} p \\ q \\ r \\ s \end{bmatrix} = \mathbf{0}.$$

`

Upon expanding, we have 1

$$p-\frac{1}{3}s=0 \quad \text{or} \quad p=\frac{1}{3}s$$

$$q-\frac{7}{6}s=0 \quad \text{or} \quad q=\frac{7}{6}s$$

$$r-\frac{2}{3}s=0 \quad \text{or} \quad r=\frac{2}{3}s,$$

the nullspace solution

$$\boldsymbol{x}=\begin{bmatrix} p \\ q \\ r \\ s \end{bmatrix}=\begin{bmatrix} \frac{1}{3} \\ \frac{7}{6} \\ \frac{2}{3} \\ 1 \end{bmatrix}s.$$

There are three pivot variables p,q,r and one free variable s. Let $s=3$, so that $p=1, q=\frac{7}{2}$ and $r=2$. We remark that this is not the only solution since there is a free variable s, the nullspace solution is infinitely many. Therefore, the chemical equation can be balanced as

$$C_2H_6+\frac{7}{2}O_2 \rightarrow 2CO_2+3H_2O.$$

Algorithm Demonstration:

C Code for reduced row echelon form:

```c
/* Reducing any mXn matrix into row echelon form */

#include<stdio.h>
#include<conio.h>
#include<math.h>
int i,j,k,a,b;
float tem;
int main()
{
    int row,col;
    float mat[80][80];
    printf("************************************************\n");
    printf("Convert any mxn matrix into Row Echelon Form\n");
    printf("Enter the number of rows : ");
    scanf("%d",&row);
    printf("Enter the number of columns : ");
    scanf("%d",&col);

    // Taking Inputs
    for(i=0;i<row;i++)
    {
        for(j=0;j<col;j++)
        {
            printf("Enter the %d,%d element : ",i+1,j+1);
            scanf("%f",&mat[i][j]);
        }
    }

    printf("Your Matrix is :: \n");
    for(i=0;i<row;i++)
    {
        for(j=0;j<col;j++)
        {
            printf("%.1f\t",mat[i][j]);
        }
        printf("\n");
    }
    // Program Logic
    for(k=0;k<row;k++)
    {

        if( (mat[k][k]) != 1)
        {
            float temp = mat[k][k];
            if(temp == 0)
                continue; // Avoiding division by zero
            for(j=0;j<col;j++)
```

```
            {
                mat[k][j] = ( (mat[k][j]) / temp );
            }
        }

        for(i=k+1;i<row;i++)
        {
            tem = mat[i][k];
            for(j=k;j<col;j++)
                {

                    mat[i][j] = mat[i][j] - ( mat[k][j] * tem );
                }

        }

        // Printing Each Step
        printf("\n**************************\n");
        if(k==row-1)
            printf("Row Echelon form is : \n\n");
        else
            printf("Step %d\n\n",k+1);
        for(a=0;a<row;a++)
        {
            for(b=0;b<col;b++)
            {
                if(mat[a][b] == -0)
                    mat[a][b] = 0; // Simply converting'-0' into '0'
                printf("%.1f\t",mat[a][b]);
            }
            printf("\n");
        }
    }
    for(int i=0;i<row;i++)
    {
        printf("\nThe unknowns are:");
        printf("X%d=%f\n",i+1,-(mat[i][col-1]));
    }

}
```

Output:

For the Equation (From example 1)

$$p\text{Fe} + q\text{O}_2 \rightarrow r\text{Fe}_2\text{O}_3.$$

$$\text{Fe}: p = 2r$$

$$\text{O}: 2q = 3r,$$

The homogeneous system of equations becomes

$$\begin{bmatrix} 1 & 0 & -2 \\ 0 & 2 & -3 \end{bmatrix} \begin{bmatrix} p \\ q \\ r \end{bmatrix} = \mathbf{0}, \quad \text{where} \quad \boldsymbol{A} = \begin{bmatrix} 1 & 0 & -2 \\ 0 & 2 & -3 \end{bmatrix}.$$

```
C:\Users\HP\ks\Kavishankar\LA>gcc rre.c

C:\Users\HP\ks\Kavishankar\LA>a
************************************************
Convert any mxn matrix into Row Echelon Form
Enter the number of rows : 2
Enter the number of columns : 3
Enter the 1,1 element : 1
Enter the 1,2 element : 0
Enter the 1,3 element : -2
Enter the 2,1 element : 0
Enter the 2,2 element : 2
Enter the 2,3 element : -3
Your Matrix is ::
1.0     0.0     -2.0
0.0     2.0     -3.0

**************************
Step 1

1.0     0.0     -2.0
0.0     2.0     -3.0

**************************
Row Echelon form is :

1.0     0.0     -2.0
0.0     1.0     -1.5

The unknowns are:X1=2.000000

The unknowns are:X2=1.500000
```

Thus substituting the unknown values into the equation we get Balanced Chemical Equation.

Conclusion

Balancing chemical reaction is not chemistry, but it is just linear algebra. This study investigates that every chemical reaction is represented by homogenous systems of linear equations only. This allows average, and even low achieving students, a real chance at success. It can remove what is often a source of frustration and failure and that turns students away from chemistry. Also, it allows the high achieving to become very fast and very accurate even with relatively difficult equations. This work presented a formal, systematic approach for balancing chemical equations. The method is based on the

Gaussian elimination especially row reduced echelon form method. The mathematical method presented in this paper was applicable to all cases in chemical reactions. The results indicated that there is no any contradiction between the various methods that were applied to balance the chemical reaction equation and the suggested approach. Balancing chemical reactions which possess atoms with fractional oxidation numbers is possible only by using mathematical methods.

$16\ MnS + 13\ As_2Cr_{10}O_{35} + 374\ H_2SO_4 \rightarrow 16\ HMnO_4 + 26\ AsH_3 + 130\ CrS_3O_{12} + 327\ H_2O$

The following chemical equation would be difficult and tedious to balance by hand. In this case a linear algebra system would be of great use. Chemists in the field today are expected to have some form of coding experience. It wouldn't be too difficult a task for most to build a linear algebra system as described above but from personal lab experience most chemists will use online chemical equation balancers. Chemical balance calculators are the easiest method to balance chemical equations because all that needs to be done is for the equation to be typed into the system and the system does the rest of the work.

References

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