Global Journal of Pure and Applied Chemistry Research
Vol.10, No.2, pp.69-76, 2022
Print ISSN: ISSN 2055-0073(Print),
Online ISSN: ISSN 2055-0081(Online)

A State-Space Method of Balancing Chemical Reactions by Using Partial-Reversible Equations Approach

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Citation: Okafor U L., Oladejo M.O., Uwa C.O., Chinyio D.T. and, Omale P. (2022) A State-Space Method of Balancing Chemical Reactions by Using Partial-Reversible Equations Approach, Global Journal of Pure and Applied Chemistry Research Vol.10, No.2, pp.69-76

ABSTRACT: *This paper describes with examples a state-space method of balancing chemical reactions using the concept of reversible equations. The method also employed the state-space analysis to show how the rows and columns of a matrix can be obtained from any given compound in a state- vector form. The proposed method employs the principle of reversible equations to demonstrate the law of conservation of mass that in any chemical reaction, atoms are not destroyed in moving from one state to another state. Considerable time and efforts are saved by the method of reversible equations when compared with the traditional echelon matrix reduction method, or the Gaussian method.*
KEYWORDS: *chemical reaction, products, reactants, reversible equations, state-space, state-vector.*

INTRODUCTION

The difference between a chemical equation and a mathematical equation has been stated by [1], and authors noting that a chemical can have a representation for a reversible and an irreversible reaction in one line. The subject of balancing chemical equations by the inspection method has been of great challenge to most students [2], equally the algebraic method has not given relive to the less gifted in mathematics as most students find it heard solving a set of simultaneous [3,4] equations. It is reported that students are at difficulty in balancing the chemical equation, while the teachers find it difficult in teaching and students find challenging to understand balancing a chemical equation [5]. The authors in [5] recommended the use of the mathematical software ..MATLAB, to circumvent the difficulty encountered in reducing a matrix to an echelon form.Andres

Prepositions

In order to implement the partial reversible equations approach, we propose as follows;

(i) **If $x = 3y$, $x=3$ and $y=1$, (3,1)**
(ii) **If $3x = 4y$, $x=4$, and $y= 3$, (4,3)**
(iii) **For a simultaneous equation such as,**
$X = 3y$, and
$3x = 4y$

Then x=3,y=1 (x,y) = (3,1) (*)
and,
3X= 4y,that means by the law of partial-reversible equations ,x =4 and y =3 (**)
The correct values for the first pair (3,1), will be obtained by multiplying the first coordinate (*) by the value of x in (**) to get 4 (3,1) = (12,4)

METHODOLOGY

In this section we will show how to use the space-state method to obtain the rows and columns of a matrix, and also represent the elements of a compound and the reactants and products of any chemical reaction in vector-space form.Next, it will be illustrated how the principle of reversible equations works. Represent the compound $x_1(NaOH) + x_2(H_2SO_4)x_1 = x3(Na2SO4) + X_4(H_20)$,in a state-space form.

, checking the number of elements involved in the chemical reaction, to get the number of rows and columns that may be needed, and here, there are 4 elements: Na,H,O, and S.

3.Example 1Balance the chemical reaction below using the method of reversible fractions;

$NaOH + H_2SO_4 \rightarrow Na_2SO4 + H_2O$
Let $x_1(NaOH) + x_2(H_2SO_4) = x_3(Na2SO4) + X_4(H_20)$

Table 1. State-Space Representation for $x_1(NaOH) + x_2(H_2SO_4)$

Na	X_1	+ 0
O	X_1	+4 X_2
H	X_1	+2 X_2
S	0	+ X_2

Next represent the right hand side as shown in Fig.2.below.

Table 2. Table 1. State-space and state- vector Representation of, $x_3(Na_2SO_4) + x_4(H_2O)$

Na	Chemical reaction below; $2X_3$ + 0	
O	$4X_3$ + X_4	
H	0 +X_4	
S	X_3 + 0	

The next concept to be explained is that of reversible fraction or mirror image, which say that, if

3y = 21x Type equation here. y=21/3

Table 3 State – Space State Vector Represention for X_1 $(NaOH)$ + $X_2(H_2SO_4)$ = X_3 (Na_2SO_4) + $X_4(H_2O)$

Na	X_1 + 0		$2X_3$ +0	
O	X_1 $+4X_2$		$4X_3$ $+X_4$	
H	X_1 + $2X_2$		0 + $2X_4$	
S	0 + X_2		X_3	

For Na, X_1 $=2X_3$ (1)

Using the principle of reversible fractions, X_1 = 2

For S, X_2 = X_3

For H , X_1 + $4X_2$ = $4X_3$ + X_4 (2)

Put X_2 = X_3 in (2), to get,

X_1 = X_4 ,since x_1 =2,therefore x_4 =2

Hence the ba; anced equation gives,

2(NaOH) + (H_2S O_4) = (Na2SO4) +2(H_20)

Worked Example2

The first 4 examples are taken from [1]

Example 1.Balance the chemical equation

Fe + O_2 → F_2O_2

Here there are two elements Fe and O

Fe + O_2 → F_2O_2

Table 3.State-Space Representation for :X_1(Fe) +X_2(O_2) = X_3(F_2O_2) (1)

Fe	X_1 +0		2 X_3
O	0+2 X_2		2 X_3

From row 1, where we have the element F, X_1 = 2 X_3,by using the principle of reversible fractions or mirror image, x_1 =2

From row 2, where we have the element O, 2 X_2 = 2 X_3, therefore, X_2 = X_3 =1

Hence,the balanced equation now becomes;

2(Fe) +(O_2) = (F_2O_2)

Example 2. Write a balanced equation for the chemical reaction below using the reversible equations and state-space method.

Fe + O_2 → F_2O_3

Let X_1(Fe) +X_2(**O_2**) = X_3(F_2O_3) (1)

Table 4.State-Space and vector- space representation for X_1(Fe) +X_2(O) = X_3(F_2O_3)

Fe	X_1 +0		2 X_3	

O	0+2 X_2		3X_3	

From row 1,where we have the element F, X_1 = 2 X_3,using the principle of reversible fractions or mirror image ,the correct value for , x_1 =2 ,and ,for the element O, 2 X_2 = 3 X_3,here,,x_2 =3 ,x_3 =2.Since x_1 = 2$x_{3,\text{the correct}}$ value for x_1 will then be giving by 2*2 = 4
The balanced equation becomes as shown in (2)

4(Fe) +2(O_3) = 2(F_2O_3) (2)

4. Balance the equation for the chemical reaction using the method of reversible fractions,
NaOH **+ $H_2S\ O_4$ → $Na_2\ SO_4$ + $H_2\ O$.**
Here,there are 4 elements Na,O, H,, and ,S ,as such four rows are needed as shown in Table 3.

Table 3

Na
O
H
S

The balanced equation is represented by (5)
X_1(NaOH **) +x_2($H_2S\ O_4$) = x_3 ($Na_2\ SO_4$) + x_4($H_2\ O$)** **(5)**
Where X_1 X_2 X_3 and X_4 ,are constants to be determined.

<u>Table 4 .State-Space and vector space for X_1(NaOH) +x_2($H_2S\ O_4$) = x_3 ($Na_2\ SO_4$) + x_4($H_2\ O$)</u>

X_1(NaOH **) +x_2($H_2S\ O_4$) = x_3 ($Na_2\ SO_4$) + x_4($H_2\ O$)**

Na	X_1 +0		**2x_3+0**
O	X_1 +4 X_2		**4 x_3 + x_4**
H	X_1 +2 X_2		**0 + 2 x_4**
S	**0+** X_2		**X_3 +0**

From row 1, considering Na element, X_1 = 2X_3 ,and using the principle of reversible fractions, X_1 =2, X_3 =1.
From 4, considering the element S, X_2 = X_3 =1
For the element O in row 2,
X_1 +4 X_2 = 4 **x_3 + x_4** **(6)**
Putting X_2 = X_3 in (6), we get (7)
X_1 +4 X_3 = 4 **x_3 + x_4** **(7)**
Hence, X_2 = X_4 **=** X_3 = **1**
Therefore, the balanced equation becomes;
2(NaOH **) + ($H_2S\ O_4$) = ($Na_2\ SO_4$) + ($H_2\ O$)** **(8)**

Obtain a balanced equation for the chemical reaction below using the method of reversible fraction.

$Na_2\ PO_4$ + Ba_2 (NO_2)$_2$ → Ba(PO_4) + $NaNO_3$

X_1 **(Na_2PO_4) +** X_2 **(Ba (NO_3)$_2$)** = X_3 **Ba(PO_4)** + X_4**($NaNO_3$)**
Where, X_1 X_2 X_3 and X_4 ,are constants to be determined

Table 5 .State-Space and vector space for X1 **(Na_2 PO4) +** X2 **(Ba (NO2)2)** = X3 **(Ba(PO4) +** X_4**($NaNO_2$)**

Na	**$2X_1$ +0**		**0+X_4**
P	**X_1+0**		**X_3 +0**
O	**$4X_1$ +$4X_2$**		**$4X_3$+$2X_4$**
Ba	**0+X_2**		**X_3 +0**
N	**0+ 2 x_2**		**0+X_4**

Using the principle of reversible fractions,
From Na : $2x_1 = x_4$, $x_1 =1, x_4 =2$, (x_1 , x_4) =(1,2)
From Ba : $x_2 = x_3$, x_3= 1
,x_2 = , (x_2, x_3) = (1, 1)

variables	X_1	X_2	X_3	X_4
value	2	2	2	4

Hence, the balanced equation is,
(Na_2PO_4) + [**Ba (NO_2)$_2$ = [Ba(PO_4)] +** 2**($NaNO_2$)**

CONCLUSION

In this paper, we have shown how to balance chemical equations using the method of reversible fractions instead of 3 century old reduction to echelon for of the Gaussian method.,or the unnecessary use of MATALAB. This new method is less time consuming and will save students the trouble of how to use any software in balancing chemical equations**.**

Example 6. By means of reversible fractions, balance the equation for the chemical reaction:

LaO_3 + B2O_3 → LaB_6 + O_2

Solution.
Let x_1 [LaO_3] +x_2 [B2O_3] = x_3[LaB_6] + x_4[O_2]
For ,La : x_1 = x_3 (1)
For O: 3X1 + 3X2 = 2X4 (2)
From B: 2X2 = 6X3, (3)
From (1) x_1 =x_3
From (3) x_3 = 2,x_2 = 6
Hence, equation (1),now gives x_1 =x_3 =2

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Using (2), $3X1 + 3X2 = 2X4$,therefore,
$3(2) + 3(6) = 2X4$
$24 = 2x_4$
$X_4 = 12$
Hence ,the balanced equation gives,

2 $[LaO_3] + 6 [B_2O_3] = 2 [LaB_6] + 12[O_2]$,
Or , $[LaO_3] + 3 [B2O_3] = [LaB_6] + 6[O_2]$,

Example 7 . By means of reversible fractions, balance the equation for the chemical reaction:
$C_7H_{16}O_4S_2 + O_2 \rightarrow CO_2 + H_2O + SO_2$
Solution.
Suppose, $x_1[C_7H_{16}O_4S_2] + x_2[O_2] = x_3[CO_2] + x_4[H_2O] + x_5[SO_2]$

Considering the elements and their coefficients, we get the equations below:
For C, $7X1 = X3$, $X3 = 7$, $X1 = 1$
For H, $16X_1 = 2X_4$, $X_4 = 8$, $X_1 = 1$
Considering the element S, $2X_1 = X_5$, $X_5 = 2$, $x_1 = 1$
From the element O, $4X_1 + 2X_2 = 2X_3 + X_4 + 2X_5$
Therefore, $4 + 2x_2 = 2*7 + 8 + 2*2$
$4 + 2x_2 = 14 + 8 + 4$
$2x_2 = 22$,hence, $x_2 = 11$
The balanced equation is now,
$(C_7H_{16}O_4S_2) + 11(O_2) = 7(CO_2) + 8(H_2O) + 2(SO_4)$
Example 8 . By means of reversible fractions, balance the equation for the following chemical reactions:

(a) $H_3BCO + H_2O \rightarrow B(OH) + + CO + H_2$
(b) $NH_3 + O_2 \rightarrow NO + H_2O$
(c) $I_2 + Na_2S_2O_3 \rightarrow NaI + Na_2S_4O_6$

Solutions.

(a) Let , $x_1(H_3BCO) + x_2(H_2O) = x_3(B(OH)) + x_4(CO) + x_5(H_2)$
For H: $3X_1 + 2X_2 = X_3 + 2X_5$ (1)
For B: $X_1 = X_3$ (2)
For C: $X_1 = X_4$ (3)
For O: $X_1 + X_2 = X_3 + x_4$ (4)
Using X_1 X_4 in (4)
We have $x_2 = x_3 = x_1$
To get x5 from (1)
$3x_1 + 2x_1 = x_1 + 2x_5$,remembering that $x_2 = x_3 = x_1$
$4x_1 = 2x_5$,then $x_1 = 2$, $x_5 = 4$
The balanced equation now becomes:
$2(H_3BCO) + 2(H_2O) = 2(B(OH)) + 2(CO) + 4(H_2)$

Or, $(H_3BCO) + (H_2O) = (B(OH)) + (CO) + 2(H_2$

(b) Let, $X_1(NH_3) + X_2(O_2) = X_3(NO)+X_4(H_2O)$

Comparing coefficients for the elements ,we obtain the following equations:

For N : $X_1 = X_3$ (1)

For H, $3X_1 = 2X_4$ (2) ,$x_4 = 3$, $X_1 = 2$,$x_3 = 2$

For O $X_2 = X_3 + X_4$ (3)

Using $X_3 = 2$,and $X_4 = 3$ in (3) we get

$2X_2 = 2 + 3$, therefore $X_2 = \frac{5}{2}$

Hence the balanced equation is;

$2(NH_3) + \frac{5}{2}(O_2) = 2(NO) + 3(H_2O)$

$4(NH_3) + 5(O_2) = 4(NO) + 6(H_2O)$

(c) Let , $X_1(I_2) + X_2(Na_2S_2O_3) = X_3(NaI)+X_4(NaS_4O_6)$

For I: $2X_1 = X_3$,,$X_3 = 2$,$X_1 = 1$

For Na: $2x_2 = x3 + x_4$

For S; $2x_2 = 4x_4$,$x_4 = 1$, $x_2 = 2$

For O : $3X_2 = 6X_4$

But $x_4 = 1$,therefore $3x_2 = 6$,x2 = 2

For Na :

$2x_2 = x_3 + x_4$

$4 = x_3 + 1$,

Or ,x3 = 3

Hence the balanced equation becomes;

$(I_2) + (Na_2S_2O_3) = 2(NaI) + 2(NaS_4O_6)$

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