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ON MATHEMATICAL METHODS TO BALANCE EQUATIONS OF CHEMICAL REACTIONS – A COMPARISON AND WAY FORWARD

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Abstract

In this study, a comparative analysis is to be conducted between different mathematical techniques to find out the best one which can be more suitable from all perspectives to balance equations of chemical reactions and to provide case-to-case recommendations for the practitioners. The linear algebra approach, linear programming approach, and integer linear programming approach have been successfully utilized for chemical equation balancing. Some chemical equations have been taken from the literature to see the performance of the above approaches. After highlighting the advantages and disadvantages of the existing approaches, some proposals for modification are presented. The proposed modifications have been worked out on all problems, and the integer solution is attained for all problems; even in cases where existing methods failed. The final recommendations on easier and better techniques have been provided. The two modified methods achieved top ratings among the existing and proposed methods.

Keywords: Mathematical methods, Chemical equations, Linear Algebra, Linear Programming, Integer Linear Programming, FLOPs, Mathematical Chemistry.

I. Introduction

Chemistry, as a subject, remains important in daily life to produce so many things through different methods and processes, while balancing chemical equations; everyone has tried to do it in different ways. The best method adopted was the trial and error method in the past [IV], [VII]. Being a participant of modern society, now a day technology has advanced rapidly day by day to do research in a well and equipped way. So, the use of compiler techniques is beneficial in the process to balance any type of chemical equation in a short time.

The equation which has some symbolic elements which react through the process to form desired products is called a chemical equation. For the researcher, this equation should remind at once, the existing form and the values of the reactants in the form shape, existence, etc. through this to get the chemical result and physical nature. The chemical equation has great importance to play its role in theoretical as well as industrial chemistry. The balancing of chemical equations was an antique problem which was one of the most highly studied topics in this process of a chemical equation. In the initial stage while involved in a chemical reaction the substance which was used in this process is called reactant but the new form of substances that produce the material are called products. The products are present in the form of a new substance with properties that are different from other reactants [XI].

The chemical equation should represent in the form of stoichiometry [I], [XIII] which was observed during a chemical reaction. This was one of the parts of chemical mathematics which is also called stoichiometry and deal with the relation of weight which is determined by chemical equations and formulas. According to this process balancing chemical equations is very important in this area, it changed in the form of a feasible as well as a natural process. The consequent equations always remain consistent since taking it as a chemical reaction. It finds a non-trivial solution and tried to become good results while obtaining it assuming its existence such an assumption can be observed as absolutely valid and does not introduce any error. After getting a result, if the reaction is feasible then find only the trivial solution i.e. all coefficients remain equal to zero.

In [XII], authors performed this to initiate the field of mathematics to propose the common issue of maintaining chemical equations. He tried to formalize a century-old problem in linear operator form to take it as a Diophantine matrix equation. There were so many others who give mathematical methods to do the process of the chemical equation which was considered remarkable in the field of chemistry since so many days in which Krishnamurthy [V] played a vital role to present this process while putting efforts in a good way. They considered some chemical equations as an elementary resource in which he offered a simple mathematical method, in which he presented the process of integer programming approach by using an inverse matrix to solve the common problem of balancing a chemical equation. He tried to apply other equations to find out mathematical results, to balance in the form of a matrix.

To support general chemistry based on ion-electron techniques to make a process for balancing chemical equations after consulting the university textbook because the best way to use it on the behalf of fundamental chemical principle [XVI], [VIII]. Most of the authors also favored other techniques which involve less algebraic manipulation which can be fruit full for attention and can be advantageous for particular classes of chemistry and chemical engineering.

Authors in [II]-[III], [VI], [VIII], [XIV]-[XVI], investigated the use of linear algebra, linear programming, and integer programming tools, like matrices, inverse matrices, a system of equations, matrix methods for the solution of linear systems and optimization to balance equations of chemical reactions. They also compared the mathematical formulation with conventional methods used in chemistry, like the ion-electron method, hit-and-trial method, valance method, etc. It was argued in [IX] that based on an intellectual level and of students and their understanding of mathematics, mathematical techniques can also be introduced in a useful way. The LINDO, MATHEMATICA, and MAPLE software were mostly used in these research studies.

In [X], authors compared the linear algebra Gauss elimination (LA-GE) and linear programming Two-phase (LP-2P) method for balancing equations of chemical reactions using MATLAB and TORA system software, respectively.

Nowadays, for a researcher, mainly working on a higher relationship of chemicals involved in hybrid and wide-scope studies, balancing the equations of chemical reactions involved, is just a side objective. Thus mathematical methods using software environment can play a vital role to help practitioners. In literature, different methods are used for balancing chemical equations. The focus of this work is on complex equations which are not easily balanced by hand calculations. We aim to provide recommendations for a simple and easy way to balance the equations among the existing methods. The recommendations can be used to efficiently balance all types of equations of chemical reactions.

The problem being considered in this work is to find a simple method to balance chemical equations using the knowledge of linear algebra “Gauss elimination approach”, “linear programming two-phase method approach”, “integer linear programming approach branch and bound method” (ILP-BB). In this work, we compare LA-GE, LP-2P, and ILP-BB techniques on some test chemical equations from the literature. We state the advantages and disadvantages of the methods to balance chemical equations. Further, we suggest proposals for modification in some techniques which fail to balance equations of chemical reactions. The proposals are worked out here, and finally, recommendations for the practitioners based on comparative analysis are shared to efficiently balance equations of chemical reactions.

II. Existing Mathematical Methods for Balancing Equations of Chemical Reactions

Here, we highlight three mathematical methods which have been used widely in past to balance equations of chemical reactions. The LA-GE and LP-2P algorithms and implementation have been discussed in detail in [X] for this purpose. Moreover, the integer linear programming approach with the branch and bound method (ILP-BB) can also be used, which is explained here as the third existing mathematical method.

In ILP-BB, first, we solve the linear programming problem by relaxing the integer conditions for the decision variables. If the obtained solution is an integer, then we cease the process, otherwise, we split the problem into two other sub-problems by looking for the largest fractional part among the variables which couldn’t be in integer values. Based on the selected variable, two constraints to make it integer lead to two further sub-problems. The procedure is repeated till all variables become integers. Thus, in the ILP-BB method, we have to use the linear programming method, LP-2P method again-and-again with full steps till the final integer solution is attained. The output of ILP-BB finally forms a binary tree of sub problems.

We explain the working of these three existing methods on two examples here for the implementation, and in the forthcoming sections, the exhaustive comparison is made on eight more, a total of ten, test equations of literature.

Example 1 [12]. $KClO_3 \longrightarrow KCl + O_2$ (1)

Example 2 [12] $CH_4 + O_2 \longrightarrow CO_2 + H_20$ (2)

To implement the LA-GE method in Examples 1-2, we begin by assigning the unknown coefficients to the terms in (1) and (2), and using the elemental balances we arrive at the matrix forms (3) and (4) for the examples (1) and (2).

$$\begin{bmatrix} 1 & -1 & 0 \\ 1 & -1 & 0 \\ 3 & 0 & -2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{3}$$

$$\begin{bmatrix} 1 & 0 & -1 & 0 \\ 4 & 0 & 0 & -2 \\ 0 & 2 & -2 & -1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{4}$$

The simplified systems (3) and (4) can be represented by the following, by converting the coefficient matrices to echelon forms, respectively:

$$\begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & -\frac{2}{3} \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \tag{5}$$

$$\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & -1 & -\frac{1}{2} \\ 0 & 0 & 1 & -\frac{1}{2} \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{6}$$

With x_2 as a free variable in (5) and x_3 in (6), we reach infinitely many solutions given in (7) and (8) for the coefficients in (1) and (2) through (5) and (6).

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = x_2 \begin{bmatrix} 1 \\ 1 \\ \frac{3}{2} \end{bmatrix}, \ for\ x_2 \in \Re - \{0\} \tag{7}$$

$$,\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = x_3 \begin{bmatrix} 1 \\ 2 \\ 1 \\ 2 \end{bmatrix}, for\ x_3 \in \Re - \{0\} \tag{8}$$

Assigning unit values to free variables, we reach the following balanced forms of (1) and (2) by the LA-GE method.

$$KClO_3 \longrightarrow KCl + \frac{3}{2}O_2 \tag{9}$$

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \tag{10}$$

It is clear to note through (9) and (10) that the LA-GE method fails in Example 1 to attain an integer solution directly, whereas it successfully attains an integer solution directly in Example 2.

To implement the LP-2P on Examples 1-2, we begin with the LP formulations of Examples 1-2, which are stated in (11) and (12), respectively.

$$\begin{aligned} &Min \quad Z = x_1 + x_2 + x_3 \\ &x_1 - x_2 + A_1 = 0 \\ &x_1 - x_2 + A_2 = 0 \\ &3x_1 - 2x_3 + A_3 = 0 \\ &And,\ x_1,\ x_2,\ x_3\ 0 \\ &x \in R^n \end{aligned} \tag{11}$$

$$\begin{aligned} &Min \quad Z = x_1 + x_2 + x_3 + x_4 \\ &x_1 - x_3 = 0 \\ &4x_1 - 2x_4 = 0 \\ &2x_2 - 2x_3 - x_4 = 0 \\ &And,\ x_1,\ x_2,\ x_3, x_4\ 0 \\ &x \in R^n \end{aligned} \tag{12}$$

The input grids for Examples 1-2 are summarized in Tables 1-2 in the TORA system software to implement LP-2P method.

Table 1. Input grid for Example-1 by LP-2P in TORA software

	x_1	x_2	x_3		
Minimize	1	1	1		
C_1	1	-1	0	=	0
C_2	1	-1	0	=	0
C_3	3	0	-2	=	0
C_4	1	0	0	>=	0
C_5	0	1	0	>=	0
C_6	0	0	1	>=	0
LB	1	1	1		
UB	Infinity	infinity	infinity		

Table 2. Input grid for Example 2 by LP-2P in TORA software

	x_1	x_2	x_3	x_4		
Minimize	1	1	1	1		
C_1	1	0	-1	0	=	0
C_2	4	0	0	-2	=	0
C_3	0	2	-2	-1	=	0
C_4	1	0	0	0	=	0
C_5	0	1	0	0	>=	0
C_6	0	0	1	0	>=	0
C_7	0	0	0	1	>=	0
LB	1	1	1	1		
UB	Infinity	infinity	infinity	infinity		

The required results were obtained in iterations 4 and 5, respectively, for Examples 1-2 in the software, and the balanced forms of (1) and (2) are:

$$KClO_3 \longrightarrow KCl + 1.5O_2 \tag{13}$$

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O \tag{14}$$

We observe that the LP-2P method also fails to get the integer solution of Example 1 directly, whereas, for Example, 2 method works fine.

The ILP formulations of the equations (1) and (2) describing Examples 1 and 2 are:

$$
\begin{aligned}
&min \quad Z = x_1 + x_2 + x_3 + S_1 + S_2 + S_3 \\
&x_1 - x_2 + S_1 = 0 \\
&x_1 - x_2 + S_2 = 0 \\
&3x_1 - 2x_3 + S_3 = 0 \\
&and,\ x_1,\ x_2,\ x_3, S_1 S_2 S_3\ 0 \\
&x \in Z^n
\end{aligned}
\tag{15}
$$

$$
\begin{aligned}
&min \quad Z = x_1 + x_2 + x_3 + x_4 \\
&x_1 - x_3 = 0 \\
&4x_1 - 2x_4 = 0 \\
&2x_2 - 2x_3 - x_4 = 0 \\
&And,\ x_1,\ x_2,\ x_3 x_4\ 0 \\
&x \in Z^n
\end{aligned}
\tag{16}
$$

In TORA software, we implemented ILP-BB on Examples 1-2, and the final output tables are given in Tables 3-4.

Table 3. Output for Example-1 by ILP-BB in TORA software

Sub problem	Z	x_1	x_2	x_3
5	7	2	2	3

Table 4. Output for Example-2 by ILP-BB in TORA software

Sub problem	Z	x_1	x_2	x_3	x_4
1	6	1	2	1	2

From Tables 3-4, it is evident that ILP-BB successfully balances the equations in Examples 1-2. But, the increased number of sub-problems for Example 1, which was 5, is the main concern in general for complex equations. The tree describing details of subproblems for Example 1 is shown in Figure 1.

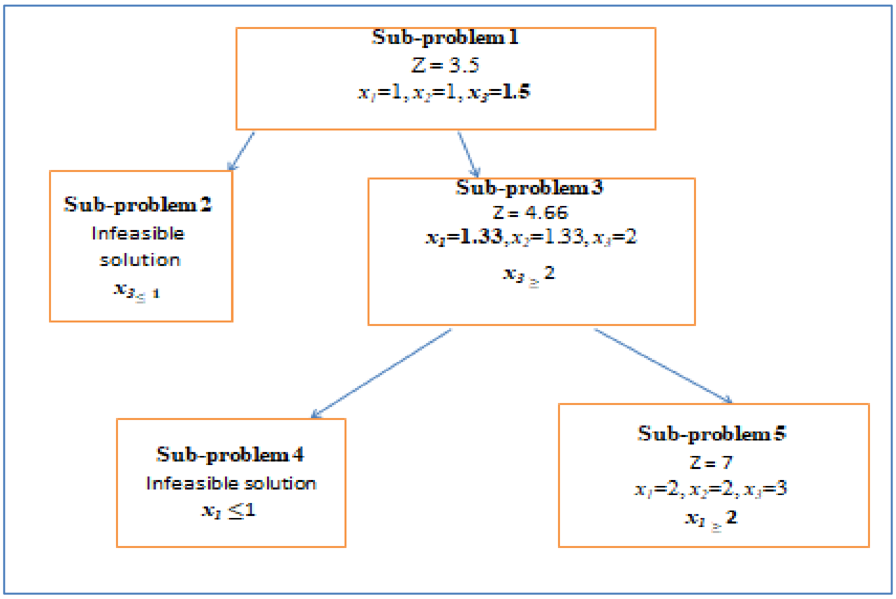

Fig 1. The detailed tree of sub-problems by ILP-BB for Example 1

The total number of floating point operations (FLOPs) in the LA-GE, LP-2P, and ILP-BB methods are given in equations (17)-(18), (19)-(20) [X] and (21)-(22) as per the present study, respectively.

$$FLOPS_{LA\text{-}GE} = FLOPS_{Echelon} + FLOPS_{Back\ Substitution} \tag{17}$$

$$Flops_{LA-GE} = \left\lceil \frac{1}{3}m^3 + m^2 \right\rceil \tag{18}$$

$$F_{LP-2P} = \left\lceil \frac{1}{2}m^2 + mn + (m-p)^2 + 2(m-p) + 4m - 1 \right\rceil \tag{19}$$

$$Flops_{LP-2P} = i \times F_{LP-2P} \tag{20}$$

$$F_{ILP-BB-j} = \left\lceil \frac{1}{2}m_j^2 + m_j n_j + (m_j - p_j)^2 + 2(m_j - p_j) + 4m_j - 1 \right\rceil, j = 1, 2, \ldots, SP \tag{21}$$

$$Flops_{ILP-BB} = \sum_{j=1}^{SP} i_j \times F_{ILP-BB-j} \tag{22}$$

$\lceil . \rceil$ denotes ceiling function.

m = number of elements/rows

n = number of coefficients/columns

p = number of pivot elements in the LP-2P method

SP = number of sub-problems

III. Proposed Modifications to LA-GE and LP-2P

It has been observed in section II that the only method from the existing ones which has a success rate of 100% was ILP-BB, whereas the other two methods: LA-GE and LP-2P failed in Example 2. The previous LA-GE and LP-2P methods can fail to acquire the integer solution to balance equations of chemical reactions. The failure cases of LA-GE and LP-2P can be addressed, and we provide some modification proposals here so that the success rate of new methods is 100%.

With the help of LA-GE, Examples 1-2 were solved through which we got the solution, but in some examples, the solution was in fraction form. The researcher is required to have integer solutions, however. We now propose using multiplying factors for the purpose to get a solution in integer form. The use of this in Example 2 with a multiplying factor of 2 produces integer coefficients 2, 2, and 3. The revised formula for FLOPs in the LA-GE-new method is defined in (23).

$$Flops_{LA-GE-NEW} = \begin{cases} \left\lceil \frac{1}{3}m^3 + m^2 \right\rceil & \text{, if solution is integer} \\ \left\lceil \frac{1}{3}m^3 + m^2 \right\rceil + n & \text{, if solution is } non-\text{integer} \end{cases} \tag{23}$$

In the formula, we see that if the solution is in integer form then the previous LA-GE flops formula is to be used. But, if the solution is a non-integer, then the second piece formula is used. We expect to look for the least common multiple in all *n* coefficients to arrive at multiplying factor, which is the added FLOPs in the existing formula.

Similarly, the LP-2P sometime produces integer solutions directly. But, in realistic situations, like example 2 where the smallest coefficient in the integer solution is more than 1, previous-LP-2P cannot provide an integer solution unless we edit the lower bound (LB), or use some other strategy.

We modify some steps, and it will be shown that the new techniques will be used to change the decimal solution into integer form. The solution is solved with the changing value of the lower bound which changes the answer in an integer value. Another way, we propose is the use of multiplying factors on the non-integer solution got by the LP-2P previous approach. So, here we propose two new strategies to compel the LP-2P to attain an integer solution. Firstly, we use the multiplying factor by using the least common multiple (LCM) of the optimal non-integer coefficients, which adds *n* to the FLOPs of the previous LP-2P approach. This modified approach is referred to as LP-2P-new1 here. The revised FLOPs formula of LP-2P-New1 is given in (24).

$$Flops_{LP-2P-NEW1} = \begin{cases} \left\lceil \frac{1}{2}m^2 + mn + (m-p)^2 + 2(m-p) + 4m - 1 \right\rceil / iteration & \text{, if solution is integer} \\ \left\lceil \frac{1}{2}m^2 + mn + (m-p)^2 + 2(m-p) + 4m - 1 \right\rceil / iteration + n & \text{, if solution is } non-\text{integer} \end{cases} \tag{24}$$

Secondly, we can compel previous LP-2P to attain an integer solution by changing the LB value, which is set to LB = 1 on default which is also a requirement in the constraints of the definition of the ILP problem. We can change the LB value from 1 to higher integers, like 2, 3, 4, … till the required integer solution arrives. But, this way, we have to solve again-an-again each new problem with changed LB by the LP-2P approach. Thus, this modified approach, referred to here as LP-2P-New2, contributes multiple FLOPs of the previous LP-2P based on the highest LB value used to produce a successful integer solution. The revised FLOPs formula for the LP-2P-NNew2 approach is given in (25).

$$Flops_{LP-2P-NEW2} = \begin{cases} \left\lceil \frac{1}{2}m^2 + mn + (m-p)^2 + 2(m-p) + 4m - 1 \right\rceil / iteration & \text{, if solution is integer} \\ \left\lceil \frac{1}{2}m^2 + mn + (m-p)^2 + 2(m-p) + 4m - 1 \right\rceil / iteration \times LB & \text{, if solution is } non-\text{integer} \end{cases} \tag{25}$$

We demonstrate in section IV that the proposed modifications LA-GE-new1, LP-2P-new1, and LP-2P-new2 have a 100% success rate in balancing equations of chemical reactions.

IV. Results and Discussion

First of all, we add eight more test equations from the literature to observe the performance of discussed methods. The other 8 equations in our sample are given below besides Examples 1-2 as in (1)-(2).

Example 3. $BaO_2 + Al \rightarrow Ba + Al_2O_3$

Example 4. $CaCN_2 + H_2O \longrightarrow CaCO_3 + NH_3$

Example 5. $K_4Fe(CN)_6 + H_2SO_4 + H_2O \rightarrow K_2SO_4 + FeSO_4 + (NH_4)_2SO_4 + CO$

Example 6. $K_4Fe(CN)_6 + KMnO_4 + H_2SO_4 \rightarrow KHSO_4 + Fe_2(SO_4)_3 + MnSO_4 + HNO_3$
$+ CO_2 + H_2O$

Example 7. $KMnO_4 + H_2SO_4 + H_2C_2O_4 \rightarrow K_2SO_4 + MnSO_4 + H_2O + CO_2$

Example 8. $CuSCN + KIO_3 + HCl \rightarrow CuSO_4 + KCl + HCN + ICl + H_2O$

Example 9. $Fe_2SiO_4 + Mg_2SiO_4 + H_2O + CO_2 \rightarrow Mg_6(Si_4O_{10})(OH)_2 + Fe_2O_3 + CH_4$

Example 10. $CrI_3 + KOH + Cl_2 \rightarrow K_2CrO_4 + KIO_3 + KCl + H_2O$

The computational details by implementing LA-GE-previous in Examples 1-10 are summarized in Table 5. The information in Table 5 has two parts in which implementation details and non-trivial solutions are discussed. The number of row operations and free variables are mentioned in a column for each example. In Example 1 four row operations are used and three variables are included because the number of reactants and products is three. One variable remained independent which is x_2. Example 1 had infinite solutions but we put the fixed value of the variable through which a specific result occurred. The result of it was found in fractions. The same method has been applied to the remaining examples as a comparison of Example 1. One free variable is necessary to be fixed in each example. Rest of the results of remaining examples is mentioned in the Table 5 and share the implementations in the same way.

We observe that except for Examples 2, 4, 5, 7, and 9 the method of LA-GE-previous fails to attain an integer solution.

In Table 6 the implementation details of LP-2P-previous are summarized and the optimal solutions are also shared. The number of iterations, coefficients, and pivot elements are mentioned in columns for each example. In Example 1, four iterations were done and three coefficients were also included because the number of reactants and products was three. The result of it was not found in integers. The same method was applied to the remaining examples as a comparison of Example 1. From Table 6, we observe that in examples 1, 3, 6, 8, and 10, the LP-2P method failed to obtain the integer solution in the natural implementation with lower bound (LB) = 1.

The computational details of the ILP-BB method in Examples 1-10 are summarized in Table 7, where a number of sub-problems are also mentioned. It can be seen from Table 7 that the ILP has succeeded in those examples as well where LA-GE-previous and LP-2P-previous, existing schemes, failed but at the cost of more sub-problems.

After using the multiplying factor concept in Examples 1, 3, 6, 8, 10, the computational details of LA-GE-new are summarized in Table 8. We can see that the LA-GE-new succeeds to find integer values of all coefficients to balance the equations. So, the success rate of LA-GE-new is 100%. The implementation details with a 100% success rate of LP-2P-new1 and LP-2P-new2 are summarized in Tables 9 and 10, respectively.

Figure 2 shows the success to a failure rate of the methods on the 10 example equations. We see that the LA-GE-Previous and LP-2P-Previous fail to produce accurate results, but the remaining approaches successfully gave the integer solution.

Using the FLOPs formulae of the methods discussed in previous section III, the FLOPs of the existing methods LA-GE-previous, LP-2P-previous, and ILP-BB are shown in Table 11. In some examples, where previous methods failed, we could not find the FLOPs. On the other hand, the FLOPs of modified methods: LA-GE-new, LP-2P-new1, and LP-2P-new2 are summarized in Table 12.

Figure 3 shows FLOPs of all methods used in this study to balance 10 example equations of chemical reactions. According to FLOPS, the values are least for the LA-GE-new, then of LP-2P-new1, then for ILP-BB, whereas LA-GE-previous and LP-2P-previous failed in examples 1, 3, 6, 8, 10.

We can compare all existing and modified approaches for balancing equations of chemical reactions from viewpoints of being manually/software adaptive, non-integer/integer solution, higher/lower FLOPs, and success/failure rate.

If we talk about manual computations, then the LA-GE echelon form can be computed manually as well as by software, but a careful look for free-variable is required in the back substitution step which should be done manually. So, LA-GE approaches, both previous and new ones, should be done manually or by manual-software combination. Specially, the back substitution should be done with care for the free variable. The LA-GE-previous cannot always assure integer solution, hence may fail to balance some equations of chemical reactions. Whereas, the proposed modification LA-GE-New can be used to successfully acquire integer solutions to balance all equations of chemical reactions. The success rate of the LA-GE-new is 100% generally, and also in the case of 10 example equations of chemical reactions used in this study from literature. On the other hand, the success rate of LA-GE-previous depends upon its ability to acquire integer solutions or not. According to the 10 examples considered in this study, the success to a failure rate of LA-GE-previous has been 50% - 50%. Based on FLOPs, the LA-GE-new and LA-GE-previous are taking equal FLOPs on examples leading to integer solution directly, whereas when LA-GE-previous fails then the LA-GE-new is still applicable and we can calculate its FLOPs. Therefore, based on FLOPs, there is a tie for both in the case where both are applicable, but generally, LA-GE-new is better as it is applicable to all equations of chemical reactions.

The LP-2P-previous method can be implemented both manually and through software. But it is recommended to use a software environment, for example, TORA or any other as this method can fully be implemented through software as well quickly and with accuracy. On the other hand, manual calculations can take a lot of time and are more prone to gross errors. The modifications LP-2P-new1 and LP-2P-new2 can also be implemented manually and by software, but the software is recommended as it can directly give accurate solutions without gross errors in the computations if the problem input parameters are well-inserted. The LP-2P-previous fails in some problems to attain the integer solution, but both new approaches always assure an integer solution. The success rate of LP-2P-new1 and LP-2P-new2 is 100% generally, which was also verified in the case of 10 example equations of chemical reactions. On the other hand, the LP-2P-previous approach may fail in acquiring integer solutions to some equations of chemical reactions, hence its failure is obvious in some cases. The success to a failure rate of the LP-2P-previous approach was the same as the LA-GE-previous as per our observation in 10 examples, which is 50% - 50%. The FLOPs in the case where all LP-2P, previous and new ones, are applicable are equal. But, in cases where LP-2P-previous fails, both new approaches can still be used with the observation that the FLOPs of LP-2P-new1 are lower than those of LP-2P-new2. Hence, the overall comparison shows that LP-2P-new1 and LP-2P-new2 are better than LP-2P-previous, whereas LP-2P-new1 is father better than LP-2P-new2.

The ILP-BB approach can be used both manually and by using software, but the use of the software is inevitably important as the former use requires a lot of time. The time is estimated as exponential, as the possibility of sub-problems multiplies the computations and execution time. Besides, ILP-BB always guarantees an integer solution and can balance the equations of all chemical reactions with a 100% success rate. The FLOPs of ILP-BB, however, are much higher than most of the other previous and new approaches discussed in this study, which were: LA-GE-previous, LA-GE-new, LP-2P-previous, LP-2P-new1. ILP-BB may bypass the previous LA-GE and LP-2P from the viewpoint of being 100% successful, but from the FLOPs point-of-view, ILP-BB cannot bypass the LA-GE-previous, LA-GE-new, LP-2P-previous, and LP-2P new1. But, the FLOPs of LP-2P-new2 are in cases higher than ILP-BB.

So, overall, we can say that LA-GE-new is the first-rated approach we can recommend for practitioners. The LP-2P-new1 takes the second place and the ILP-BB the third and LP-2P-new2 the fourth rating among all methods having a 100% success rate.

Table 5. Implementation details of LA-GE-previous for Examples 1-10

Test Equations	LA-GE-previous Implementation details		Non Trivial Solutions for Variable x_i										Success
	Row Operations Used	Free Variable	1	2	3	4	5	6	7	8	9	10	
1	4	2nd	1	1	$\frac{3}{2}$	-	-	-	-	-	-	-	NO
2	4	3rd	1	2	1	2	-	-	-	-	-	-	YES
3	3	3rd	1	$\frac{4}{3}$	1	$\frac{2}{3}$	-	-	-	-	-	-	NO
4	6	3rd	1	3	1	2	-	-	-	-	-	-	YES
5	17	1st	1	6	6	2	1	3	6	-	-	-	YES
6	20	5th	2	$\frac{122}{5}$	$\frac{299}{5}$	$\frac{162}{5}$	1	$\frac{122}{5}$	12	12	$\frac{185}{5}$	-	NO
7	14	4th	2	3	5	1	2	8	10	-	-	-	YES
8	15	8th	$\frac{4}{5}$	$\frac{7}{5}$	$\frac{14}{5}$	$\frac{4}{5}$	$\frac{7}{5}$	$\frac{4}{5}$	$\frac{7}{5}$	1	-	-	NO
9	11	1st	4	12	18	1	4	4	1	-	-	-	YES
10	12	7th	1	26	$\frac{21}{2}$	1	3	21	13	-	-	-	NO

Table 6. Implementation details of LP-2P-previous for Examples 1-10

Test Equations	LP-2P-previous Implementation Details			Optimal Minimal Solution for Variable x_i										Success
	Iterations	coefficients	Pivots	1	2	3	4	5	6	7	8	9	10	
1	4	3	2	1	1	1.5	-	-	-	-	-	-	-	NO
2	5	4	2	1	2	1	2	-	-	-	-	-	-	YES
3	5	4	3	1	1.33	3	0.66	-	-	-	-	-	-	NO
4	5	4	3	1	3	1	2	-	-	-	-	-	-	YES
5	9	7	7	1	6	6	2	1	3	6	-	-	-	YES
6	10	9	8	2	24.4	59.8	32.4	1	24.5	12	12	37.6	-	NO
7	8	7	6	2	3	5	1	2	8	10	-	-	-	YES
8	8	8	7	1	1.75	3.50	1	1.75	1	1.75	1.25	-	-	NO
9	8	7	6	4	12	18	1	4	4	1	-	-		YES
10	8	7	6	1	26	10.5	1	3	21	13	-	-	-	NO

Table 7. Implementation details of ILP-BB method on Examples 1-10

Test Equations	ILP-BB implementation details			Optimal Minimal Solution for Variable x_i							Success			
	Number of reactants	Number of products	Number of Sub-problems	1	2	3	4	5	6	7	8	9	10	
1	1	2	5	2	2	3	-	-	-	-	-	-	-	YES
2	2	2	1	1	2	1	2	-	-	-	-	-	-	YES

3	2	2	7	3	4	3	2	-	-	-	-	-	-	YES
4	2	2	1	1	3	1	2	-	-	-	-	-	-	YES
5	3	4	1	1	6	6	2	1	3	6	-	-	-	YES
6	3	6	23	10	122	299	162	5	122	60	60	188	-	YES
7	3	4	1	2	3	5	1	2	8	10				YES
8	3	5	13	4	7	14	4	7	4	7	5			YES
9	4	3	1	4	12	18	1	4	4	1				YES
10	3	4	5	2	52	21	2	6	42	26				YES

Table 8. Implementation details of LA-GE-new on Examples 1-10

Test Equations	LA-GE-new Implementation details			Non Trivial Solutions for Variable xi									Success
	Row Operations Used	Free Variable	Multiplying factor	1	2	3	4	5	6	7	8	9	
1	4	2nd	2	2	2	3	-	-	-	-	-	-	YES
2	4	3rd	------	1	2	1	2	-	-	-	-	-	YES
3	3	3rd	3	3	4	3	2	-	-	-	-	-	YES
4	6	3rd	-----	1	3	1	2	-	-	-	-	-	YES
5	17	1st	------	1	6	6	2	1	3	6	-	-	YES
6	20	5th	5	10	122	299	162	5	122	60	60	185	YES
7	14	4th	------	2	3	5	1	2	8	10	-	-	YES
8	15	8th	5	4	7	14	4	7	4	7	5	-	YES
9	11	1st	2	4	12	18	1	4	4	1	-	-	YES
10	12	7th	-----	2	52	21	2	6	42	26	-	-	YES

Table 9. Implementation details of LP-2P-new1 on Examples 1-10

Test Equations	LP-2P-new1 Implementation details				Optimal Minimal Solutions for Variable xi									Success
	Iterations	Coefficients	Pivots	Multiplying factor	1	2	3	4	5	6	7	8	9	
1	4	3	2	2	2	2	3	-	-	-	-	-	-	YES
2	5	4	2	------	1	2	1	2	-	-	-	-	-	YES
3	5	4	3	3	3	4	3	2	-	-	-	-	-	YES
4	5	4	3	-----	1	3	1	2	-	-	-	-	-	YES
5	9	7	7	------	1	6	6	2	1	3	6	-	-	YES
6	10	9	8	5	10	122	299	162	5	122	60	60	185	YES
7	8	7	6	------	2	3	5	1	2	8	10	-	-	YES
8	8	8	7	5	4	7	14	4	7	4	7	5	-	YES
9	8	7	6	------	4	12	18	1	4	4	1	-	-	YES
10	8	7	6	2	2	52	21	2	6	42	26	-	-	YES

Table 10. Implementation details of LP-2P-new2 on Examples 1-10

Test Equations	LP-2P-new2 Implementation details				Optimal Minimal Solutions for Variable xi									Success
	Iterations	Coefficients	Pivots	LB	1	2	3	4	5	6	7	8	9	
1	4	3	2	2	2	2	3	-	-	-	-	-	-	YES
2	5	4	2	------	1	2	1	2	-	-	-	-	-	YES
3	5	4	3	2	3	4	3	2	-	-	-	-	-	YES
4	5	4	3	-----	1	3	1	2	-	-	-	-	-	YES
5	9	7	7	------	1	6	6	2	1	3	6	-	-	YES
6	10	9	8	5	10	122	299	162	5	122	60	60	185	YES
7	8	7	6	------	2	3	5	1	2	8	10	-	-	YES

8	8	8	7	4	4	7	14	4	7	4	7	5	-	YES
9	8	7	6	------	4	12	18	1	4	4	1	-	-	YES
10	8	7	6	2	2	52	21	2	6	42	26	-	-	YES

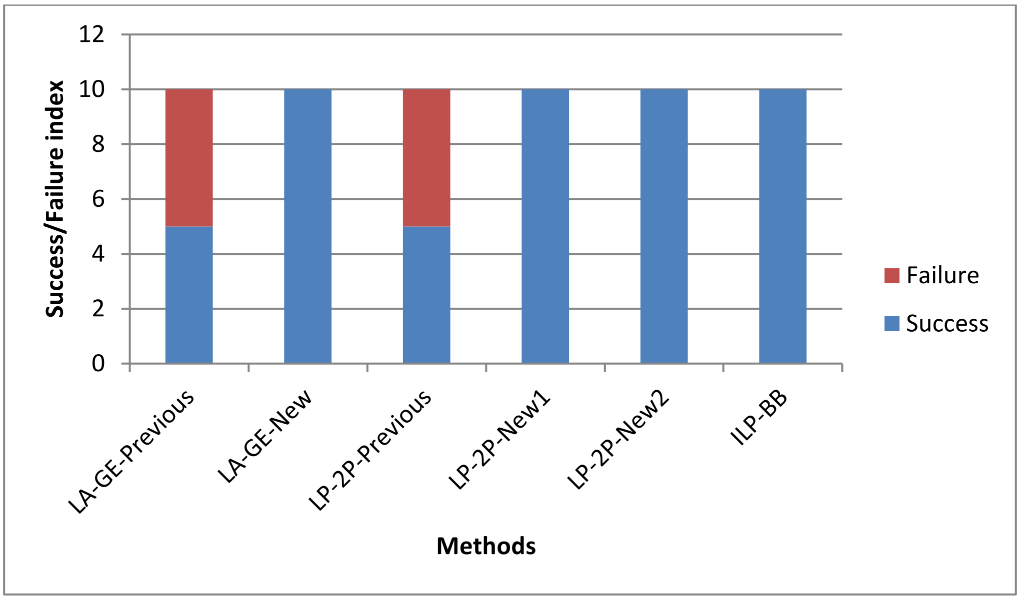

Fig. 2. Success and Failure rates of methods based on Examples 1-10

Table 11. FLOPs in existing methods for Examples 1-10

Example	Number of reactant	Number of product	LA-GE approach	LP-2P approach	ILP-BB approach
1	1	2	FAILS	FAILS	602
2	2	2	25	140	140
3	2	2	FAILS	FAILS	1812
4	2	2	58	300	300
5	3	4	164	909	909
6	3	6	FAILS	FAILS	73642
7	3	4	121	664	664
8	3	5	FAILS	FAILS	17168
9	4	3	121	664	664
10	3	4	FAILS	FAILS	2763

Table 12. FLOPs in modified methods for Examples 1-10

Example	Number of reactant	Number of product	LA-GE-new	LP-2P-new1	LP-2P-new2
1	1	2	21	115	1204
2	2	2	25	140	140
3	2	2	29	144	3624
4	2	2	58	300	300
5	3	4	164	909	909
6	3	6	261	1359	3638210
7	3	4	121	664	664
8	3	5	243	1088	85840
9	4	3	121	664	664
10	3	4	128	671	5526

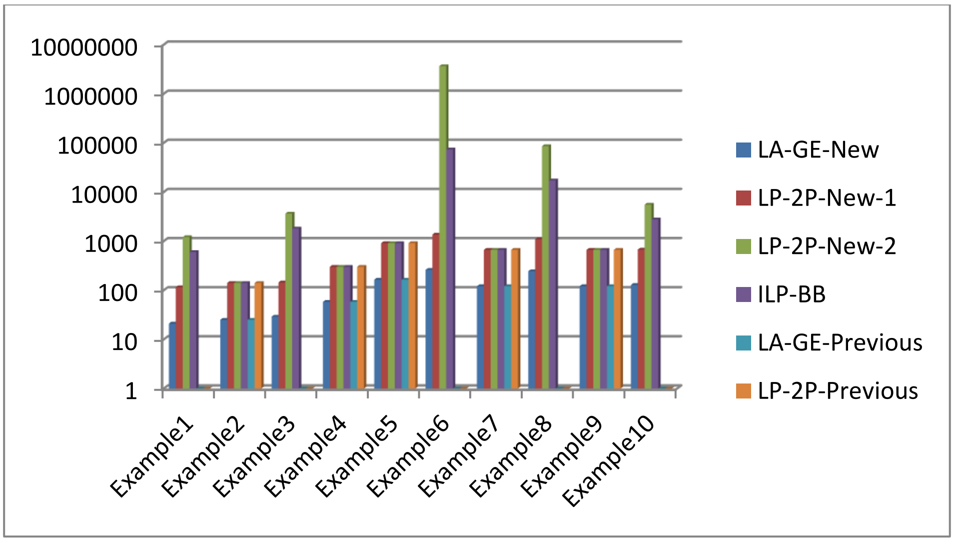

Fig.3. FLOPs comparison of existing and proposed methods for Examples 1-10.

V. Conclusion

Different mathematical methods were discussed for balancing equations of chemical reactions. Exhaustive comparisons of three different existing approaches/techniques on test equations, which were based on literature, were made using the computational procedure, general form, implementations, and advantages, disadvantages of all approaches were explained and examined. It was found that among the existing previous techniques: LA-GE, LP-2P, and ILP-BB, the ILP-BB had a 100% success rate for balancing the equation of chemical reaction, but it requires a lot higher FLOPs because of an increased number of sub-problems in some cases. The LA-GE-previous and LP-2P-previous failed to acquire integer solutions in some cases, so cannot be recommended to practitioners in the usual form. We also attempted to modify the LA-GE and LP-2P approaches by adding some working strategies to assure the integer solution to balance any equation of the chemical reaction. The modified LA-GE-new and LP-2P-new1 use the concept of multiplying factors to assure the integer solution. Whereas, amending lower bound values was suggested in form of modified LP-2P-new2. All the proposed modifications exhibit a 100% success rate. The revised formula of FLOPs was developed and explained for the new approaches. The LA-GE-new approach can be used manually or in a bridged manual-software environment, and it was shown to be a direct and more reliable technique than any other technique which is the best method for balancing the equation of the chemical reaction. Secondly, LP-2P-new-1 is the best approach, thirdly ILP-BB approach and last LP-2P-New-2 is a better approach. Finally, it was recommended to use some software environment on the computer to balance equations arising from complex chemical reactions. A chemistry scholar requires easy technique and is approachable to gain exact solutions. All the above requirements have been fulfilled by the proposed techniques and existing ILP-BB method, and we were able to solve too difficult equations as well as lengthy equations.

Conflict of Interest:

There was no relevant conflict of interest regarding this paper.

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