

Automated Balancing of Complex Redox Reactions Using MAPLE Software and Linear Algebra

Ghala S. Alharbi

*Faculty of Computing and Information Technology
King Abdulaziz University, Rabigh
Saudi Arabia*

Abstract

Balancing chemical equations is a fundamental principle in chemistry that ensures mass and charge conservation during chemical processes. Simple reactions can be balanced manually, but more complex redox processes necessitate systematic and accurate methods. Classical methods of balancing chemical equations sometimes use trial-and-error or algebraic techniques, which can be time-consuming and prone to error. This study aims to demonstrate how linear algebra-based approaches in conjunction to MAPLE software can simplify and speed up the balancing of complex redox reactions, resulting in a more systematic and accurate approach. To generate solutions, we employ matrix representations of chemical equations with MAPLE software. The algorithm gives coefficients to reactants and products in sequence, ensuring mass and charge balance. In comparison to manual balancing, the recommended approach greatly decreases calculation time while improving accuracy. Computational technologies simplify the process, making it more accessible to students, teachers, and researchers. By integrating chemistry, mathematics, and programming, this study highlights the importance of multidisciplinary approaches in advancing chemical education and research. The findings highlight the potential of computational methods in simplifying difficult chemical challenges, opening the path for further research in this area.

1. Introduction

Balancing equations for chemicals is a vital component of chemistry since this ensures that chemical processes obey the law of mass conservation. This principle states that the number of atoms for each substance must be consistent across the reactants as well as the outcomes of a reaction. While simple equations may frequently be balanced by hand, complicated reactions with several components and elaborate stoichiometries create substantial difficulties.

To handle this level of complexity, mathematical methods including linear algebra offer a systematic and efficient answer. Chemists can use systematic approaches to find answers to the chemical balancing

problem by translating it into a system of linear equations, each representing an element's conservation. Linear algebra not just simplifies the procedure, but it also ensures that the answers are true and can handle complex cases like fractional stoichiometry and large-scale reactions.

2. Literature Review

In the past few decades, there has been considerable number of studies into employing linear algebra for balancing chemical equations. Fogler [1] established the use of linear systems to simulate conservation principles in chemical processing methods, which was a seminal paper. His approach established a way for incorporating mathematical tools into chemical problem solving. Hamid [2] described a structured and systematic approach to balance chemical reactions formulas. The technique is suitable for chemical processes involving atoms having fractional oxidation values. The chemical equations became balanced by converting them into mathematical systems of linear equations and are finally resolved utilizing the Gauss elimination technique.

Johar [3] discovered gaps in current techniques in balancing chemical interaction equations. His investigation was aimed at disputing prior findings that suggested linear equation systems might be utilized in balancing chemical reactions. The investigation applied Gauss and Gauss-Jordan eliminating to deal with linear equation systems modeling chemical reactions and discovered that this method would handle any kind of chemical reaction. Sen et al. [4] introduced two approaches to automatically balancing chemical equations: integer linear programs (ILP) and integer nonlinear programs (INP). The INP method has been evaluated on a variety of chemical equations and proved to be extremely effective at balancing most of them. The INP algorithm can assess the possibility of a novel chemical reaction, balancing the equation, and determining if there are several linearly independent solutions.

Kafi and Abdillah [5] demonstrated strategies to balance the reactions of chemicals by employing

linear systems. All the cases demonstrate that linear systems are an appropriate approach to the problem of balancing chemical reactions. The basic row operations performed to an augmented matrix. The accuracy of the manual calculations for each of the instances provided has been validated by the MATLAB software.

Kumar [6] studied software developed on computers for balancing chemical equations. Six of the 13 approaches evaluated are matrix-based:

- two are active programs,
- a stand-alone system,
- an algorithm in Basic,
- depends on concept engineering,
- written in HyperCard, and
- created for the World Wide Web.

Besides balancing chemical equations, other features include:

- determining the number of distinct chemical processes,
- calculating production,
- forecasting mass connections,
- and balancing rare reactions.

Research and development difficulties are addressed.

Croteau et al. [7] illustrated how matrix algebra can model chemical stoichiometry effectively, while Rao and Aris [8] revisited the concept of detailed and complex balancing in chemical networks.

More recently, Sharma and Sharma [9] introduced mathematical programming techniques capable of automating the balancing of reactions with multiple constraints. Niaz and Fernandez [10] further demonstrated how matrices could be used not only to balance reactions but also to model their implications.

Othman and Ali [11] emphasized the broader role of applied mathematics in chemical equation analysis. Collectively, these studies validate the integration of symbolic computation platforms like MAPLE, which automate and scale the balancing process with accuracy and pedagogical clarity. These studies demonstrate the increasing significance of mathematical techniques and computer programming in chemistry. Chemists can manage complex reactions with improved accuracy and efficiency by utilizing linear algebra, opening the path for future advances in both theoretical and applied chemistry.

The article investigates the implementation of MAPLE programming based on linear algebra in balancing complex chemical equations. This approach

benefits both fields by linking chemistry and computer programming, providing excellent tools for researchers, instructors, and practitioners.

3. Methodology

Based on linear algebra, two examples will be discussed. In the first example, the solutions will be obtained manually by applying the system of linear equations. The solutions of the second example will be generated with the aid of MAPLE software.

4. Balancing Simple Chemical Redox Reactions Via Linear System

The chemical equation, or reaction equation, is a description of a chemical process by a group of symbols and chemical formulas that represent the reactants, products, and electrons gained or lost from the atoms of the reacting elements [1]. The chemical equation balancing is a necessary process when studying one of the chemistry branches or dealing with any of its fields and addressing one of its interactions. Mathematical representation is a theoretical framework that utilizes arithmetic language for describing the behavior of a system. Mathematical models can be used in many fields, such as chemistry, physics, biology, engineering, economics, and many types of sciences. The principle of mathematical modeling will be applied to chemical equations to facilitate balancing them. The method will be as follows:

First: Identify the reactants and products in the chemical equation.

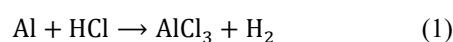
Second: write the unbalancing equation.

Third: For balancing the equation, we enter the unknowns and multiply the reactants and products to get the equation in the new form.

Fourth: Transform the chemical equation into a mathematical equation.

Fifth: Solve the equation algebraically if the system is simple and by Maple programming if the linear system is complex.

Example 1. Consider the unbalanced redox reaction between aluminum (Al) and hydrochloric acid (HCl)



Identify the reactants:

Al, Cl, H

Multiply the unknowns by the reactants and products:



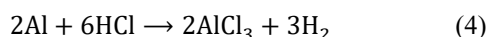
Convert the chemical equation into a system of linear mathematical equation:

$$\begin{array}{ll} \text{Al:} & x_1 = x_3 \\ \text{Cl:} & x_2 = 3x_3 \\ \text{H:} & x_2 = 2x_4 \end{array} \quad (3)$$

This results in a system of three equations with four unknowns, representing an underdetermined linear system. By choosing a value for one free variable, such as $x_3 = 2$, the remaining variables can be determined as

$$x_1 = 2, x_2 = 6, \text{ and } x_4 = 3$$

By substituting the values of the unknowns in the unbalanced chemical equation, we obtain the balanced equation as follows:



5. Balancing Simple and Complex Redox Reactions using MAPLE Programming

Solving chemical equations with the linear system technique, one potential issue is caused by the existence of infinitely many solutions in certain cases. This problem arises from the basic characteristics of linear systems and the nature of chemical equations. For chemical reactions with many reactants and products, the system of equations can grow enormous and rely heavily on normalization procedures. Ensuring that the correct subset of solutions (minimum integer coefficients) is selected becomes more difficult and time-consuming. Even though chemical equations typically require integers, the general solution to a linear system may incorporate fractional coefficients. These fractions must be scaled to obtain the smallest whole-number result, which adds an extra step. Scaling fractional solutions appropriately can generate errors, especially in complicated systems with large coefficients.

For these reasons, specialized software like Maple provides more efficient and accurate solutions tailored to chemical requirements. Maple is a robust mathematical software program that specializes in symbolic computation, making it ideal for automating activities such as balancing chemical equations.

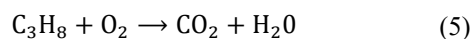
Maple can automatically set up and solve the underlying linear system, reducing the risk of human error. The process is significantly faster, especially for complex reactions with multiple reactants and products. Maple can handle fractional coefficients, constraints (like only integer coefficients), or optimization for specific conditions (e.g., minimal coefficients) – (see Table 1).

Table 1. Key MAPLE Commands Used

Command	Purpose
restart	Clears MAPLE memory
with(linalg)	Loads linear algebra tools
solve(eqs, vars)	Solves system of equations symbolically
eval(expr, subs)	Substitutes variables
ilcm(...)	Finds least common multiple of denominators
printf(...)	Formats and displays the final balanced equation

Example 2. Combustion of Propane (C_3H_8)

In this example, we demonstrate the balancing of a basic combustion reaction involving propane (C_3H_8). It illustrates a straightforward system where the number of atoms of carbon, hydrogen, and oxygen must be conserved. MAPLE is used here in a direct solve-evaluate-print method, making it ideal for introductory-level automation. The unbalanced reaction [12]:

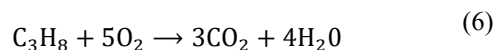


MAPLE Code

```
restart;
with(LinearAlgebra);
eqs := [3*x1 = x3, 8*x1 = 2*x4, 2*x2 = 2*x3 + x4];
sol := solve(eqs, {x2, x3, x4});
x1 := 1;
x2 := eval(x2, sol);
x3 := eval(x3, sol);
x4 := eval(x4, sol);
printf("Balanced Equation:\n%d C3H8 + %d O2 ->
%d CO2 + %d H2O\n", x1, x2, x3, x4);
```

Result

Balanced Equation:

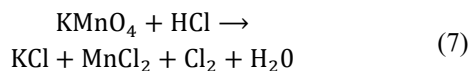


This example highlights the use of symbolic solving with substitution, where the system is solved in terms of a single variable and later evaluated with integer values. This approach is simple and readable for students and early learners in computational chemistry.

Example 3. Potassium Permanganate and Hydrochloric Acid Reaction

The following example involves a moderately complex redox reaction between potassium permanganate and hydrochloric acid. This case

demonstrates a second MAPLE programming technique where the system is solved symbolically and values are scaled to avoid fractions. The code also includes integer conversion and negative coefficient correction. The unbalanced reaction [12]:

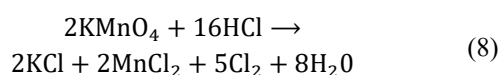


MAPLE Code:

```
restart;
with(LinearAlgebra);
eqs := [x1 = x3, x1 = x4, x2 = x3 + 2*x4 + 2*x5, x2 = 2*x6, 4*x1 = x6];
sol := solve(eqs, {x2, x3, x4, x5, x6});
x1 := 1;
x2 := eval(x2, sol);
x2 := eval(x2, sol);
x3 := eval(x3, sol);
x4 := eval(x4, sol);
x5 := eval(x5, sol);
x6 := eval(x6, sol);
lcm_val := ilcm(denom(x2), denom(x3), denom(x4),
denom(x5), denom(x6));
x1 := x1*lcm_val;
x2 := x2*lcm_val;
x3 := x3*lcm_val;
x4 := x4*lcm_val;
x5 := x5*lcm_val;
x6 := x6*lcm_val;
printf("Balanced Equation:\n%d KMnO4 + %d HCl -
> %d KCl + %d MnCl2 + %d Cl2 + %d H2O\n", x1,
x2, x3, x4, x5, x6);
```

Result:

Balanced Equation:

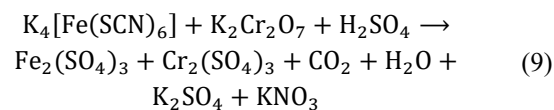


Unlike the second example, this method includes conditional scaling and manual expression evaluation, showcasing MAPLE's flexibility. Multiple coding styles can be adopted depending on the user's goal—whether to minimize coding effort, maximize clarity, or handle complex symbolic systems.

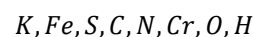
Example 4. Redox Between Potassium Ferrocyanide and Potassium Dichromate

Consider the next unbalanced redox reaction [13] between potassium ferrocyanide and potassium dichromate in an acidic medium. This example involves multiple species including polyatomic ions

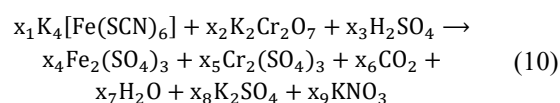
and gaseous products. MAPLE's symbolic algebra handles the complexity of simultaneous conservation constraints effectively, ensuring stoichiometric accuracy without resorting to empirical balancing.



Identify the reactants:



Multiply the unknowns with the reactants and products:



Transform the chemical equation into a linear mathematic equation system:

$$\text{K: } 4x_1 + 2x_2 = 2x_8 + x_9$$

$$\text{Fe: } x_1 = 2x_4$$

$$\text{S: } 6x_1 + x_3 = 3x_4 + 3x_5 + x_6$$

$$\text{C: } 6x_1 = x_6$$

$$\text{N: } 6x_1 = x_9 \quad (11)$$

$$\text{Cr: } 2x_2 = 2x_5$$

$$\text{O: } 7x_2 + 4x_3 = 12x_4 + 12x_5 + 2x_6 + x_7 +$$

$$4x_8 + 3x_9$$

$$\text{H: } 2x_3 = 2x_7$$

MAPLE Code

Restart:

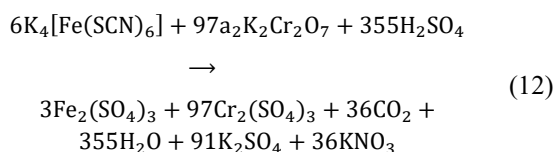
```
with(LinearAlgebra);
eqs := [4*x1 + 2*x2 = 2*x8 + x9, x1 = 2*x4, 6*x1 +
x3 = 3*x4 + 3*x5 + x6, 6*x1 = x6, 6*x1 = x9, 2*x2 =
2*x5, 7*x2 + 4*x3 = 12*x4 + 12*x5 + 2*x6 + x7 +
4*x8 + 3*x9, 2*x3 = 2*x7];
sol := solve(eqs, {x2, x3, x4, x5, x6, x7, x8, x9});
x1 := 1;
x2 := eval(x2, sol);
x3 := eval(x3, sol);
x4 := eval(x4, sol);
x5 := eval(x5, sol);
x6 := eval(x6, sol);
x7 := eval(x7, sol);
x8 := eval(x8, sol);
x9 := eval(x9, sol);
lcm_val := ilcm(denom(x2), denom(x3), denom(x4),
denom(x5), denom(x6), denom(x7), denom(x8),
denom(x9));
```

```

x1 := x1*lcm_val;
x2 := x2*lcm_val;
x3 := x3*lcm_val;
x4 := x4*lcm_val;
x5 := x5*lcm_val;
x6 := x6*lcm_val;
x7 := x7*lcm_val;
x8 := x8*lcm_val;
x9 := x9*lcm_val;
printf("Balanced Equation:\n%d K4[Fe(SCN)6] + %d
K2Cr2O7 + %d H2SO4 -> %d Fe2(SO4)3 + %d
Cr2(SO4)3 + %d CO2 + %d H2O + %d K2SO4 + %d
KNO3\n", x1, x2, x3, x4, x5, x6, x7, x8, x9);

```

Result:



MAPLE Code

```

Restart:
with(linalg):
A := Matrix([[4, 2, 0, 0, 0, 0, 0, -2, -1],
[1, 0, 0, -2, 0, 0, 0, 0, 0],
[6, 0, 1, -3, -3, 0, 0, -1, 0],
[6, 0, 0, 0, 0, -1, 0, 0, 0],
[6, 0, 0, 0, 0, 0, 0, 0, -1],
[0, 2, 0, 0, -2, 0, 0, 0, 0],
[0, 7, 4, -12, -12, -2, -1, -4, -3],
[0, 0, 2, 0, 0, 0, -2, 0, 0]]):
gaussjrd(A);

```

Result:

$$\begin{bmatrix}
 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{6} \\
 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{97}{36} \\
 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -\frac{355}{36} \\
 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -\frac{1}{12} \\
 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\frac{97}{36} \\
 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 \\
 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -\frac{355}{36} \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -\frac{91}{36}
 \end{bmatrix} \quad (13)$$

Alternatively, the Gauss-Jordan elimination can be used to solve the system of linear equations for balancing chemical reactions. Gauss-Jordan is a method for solving systems of linear equations by transforming the augmented matrix into reduced row

echelon form. Therefore, we can approach this problem using Gauss-Jordan elimination in Maple to balance the reaction (Eq. (9)).

We will create an augmented matrix for the system of equations (Eq. (11)) in Maple in then apply the Gauss-Jordan command.

The last column represents the multiplied coefficient with x_9 . Next, we take the least common multiple for the denominators of fractions and we assume that $x_9 = 36$.

After compensation, the solution will be as follows:

$$\begin{aligned}
 x_1 = 6, x_2 = 97, x_3 = 355, x_4 = 3, x_5 = 97, \\
 x_6 = 36, x_7 = 355, x_8 = 91, x_9 = 36.
 \end{aligned} \quad (14)$$

Therefore, it leads to the same balanced chemical reaction in Eq. (12).

It is worth mentioning that when solving the system of equations for chemical reaction balancing using symbolic methods (such as Gauss-Jordan elimination in MAPLE), it is possible for some stoichiometric coefficients to appear as negative values. This variation does not indicate an error in the mathematical process or chemical logic. Instead, it reflects the algebraic flexibility of the system, where the side of the equation (reactants or products) is not inherently fixed by the matrix formulation.

A negative coefficient simply implies that the corresponding species should be moved to the opposite side of the reaction equation. For example, a substance originally placed among the products with a negative coefficient should instead appear on the reactant side with a positive coefficient of the same magnitude. This adjustment ensures the physical validity of the balanced chemical equation, in which all stoichiometric coefficients must be non-negative integers. This behavior typically arises from the presence of free variables, underdetermined systems, or arbitrary ordering of species during matrix construction.

It is standard practice in computational chemistry to normalize all coefficients after solving, scale them to the smallest set of positive integers, and then correctly position the species based on the sign of the result.

Final chemical equations must always have positive integer coefficients. Any negative output from symbolic computation must be interpreted and rearranged accordingly before presenting the final balanced reaction.

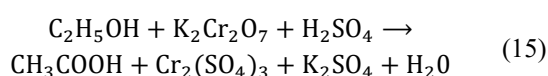
Example 5. Oxidation of Ethanol with Dichromate in Acidic Medium

This example demonstrates the oxidation of an organic compound—ethanol ($\text{C}_2\text{H}_5\text{OH}$)—by an inorganic oxidizing agent—potassium dichromate ($\text{K}_2\text{Cr}_2\text{O}_7$)—in the presence of sulfuric acid (H_2SO_4).

The products include acetic acid (CH_3COOH), chromium(III) sulfate ($\text{Cr}_2(\text{SO}_4)_3$), potassium sulfate (K_2SO_4), and water.

The reaction is commonly studied in analytical and organic chemistry due to its relevance in alcohol oxidation, and it serves as a model case for balancing redox reactions involving both organic molecules and polyatomic ions. The complexity arises from managing multiple oxidation states and polyatomic groups like sulfate. MAPLE is used here to symbolically construct and solve the stoichiometric system, ensuring that the balance of each element is achieved with precision, even in the presence of complex species.

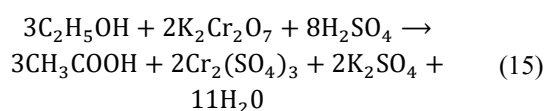
Unbalanced Reaction [12]:



MAPLE Code

```
restart;
with(linalg);
eqs := [2*x1 = 2*x4, 6*x1 + 2*x3 = 4*x4 + 2*x7, x1
+ 7*x2 + 4*x3 = 2*x4 + 12*x5 + 4*x6 + x7, 2*x2 =
2*x5, 2*x2 = 2*x6, 3*x5 + x6 = x3];
sol := solve(eqs, {x2, x3, x4, x5, x6, x7});
x1 := 1;
x2 := eval(x2, sol);
x3 := eval(x3, sol);
x4 := eval(x4, sol);
x5 := eval(x5, sol);
x6 := eval(x6, sol);
x7 := eval(x7, sol);
lcm_val := ilcm(denom(x2), denom(x3), denom(x4),
denom(x5), denom(x6), denom(x7));
x1 := x1*lcm_val;
x2 := x2*lcm_val;
x3 := x3*lcm_val;
x4 := x4*lcm_val;
x5 := x5*lcm_val;
x6 := x6*lcm_val;
x7 := x7*lcm_val;
printf("Balanced Equation:\n%d C2H5OH + %d
K2Cr2O7 + %d H2SO4 -> %d CH3COOH + %d
Cr2(SO4)3 + %d K2SO4 + %d H2O\n", x1, x2, x3,
x4, x5, x6, x7);
```

Balanced Equation:



The ethanol–dichromate redox reaction highlights the challenges of balancing redox equations that involve both organic compounds and polyatomic ions (see Table 2). Chromium in $\text{K}_2\text{Cr}_2\text{O}_7$ is reduced

Table 2. Summary of Balanced Redox Reactions

Example	Reaction
1	$2\text{Al} + 6\text{HCl} \rightarrow 2\text{AlCl}_3 + 3\text{H}_2$
2	$\text{C}_3\text{H}_8 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O}$
3	$2\text{KMnO}_4 + 16\text{HCl} \rightarrow 2\text{KCl} + 2\text{MnCl}_2 + 5\text{Cl}_2 + 8\text{H}_2\text{O}$
4	$6\text{K}_4[\text{Fe}(\text{SCN})_6] + 97\text{a}_2\text{K}_2\text{Cr}_2\text{O}_7 + 355\text{H}_2\text{SO}_4 \rightarrow 3\text{Fe}_2(\text{SO}_4)_3 + 97\text{Cr}_2(\text{SO}_4)_3 + 36\text{CO}_2 + 355\text{H}_2\text{O} + 91\text{K}_2\text{SO}_4 + 36\text{KNO}_3$
5	$\text{C}_2\text{H}_5\text{OH} + \text{K}_2\text{Cr}_2\text{O}_7 + \text{H}_2\text{SO}_4 \rightarrow \text{CH}_3\text{COOH} + \text{Cr}_2(\text{SO}_4)_3 + \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$

from +6 to +3, while ethanol is oxidized from an alcohol to a carboxylic acid. This system includes seven unique elements—C, H, O, Cr, K, and S—which makes manual balancing error-prone, particularly when sulfate ions are distributed among multiple product species. MAPLE effectively manages this complexity by symbolically solving a system of linear equations based on atomic conservation.

The software's ability to scale fractional solutions into integer coefficients eliminates the guesswork and repetitive iterations that often accompany traditional balancing methods. The result is a fully balanced redox reaction that adheres to both mass and charge conservation principles, presented in a format ready for use in laboratory, educational, or analytical contexts (see Table 2).

6. Avoiding Errors in Redox Balancing: MAPLE's Role

Manually balancing redox reactions, especially those involving polyatomic ions, transition metals, and organic compounds—as shown in Examples 4 and 5—can be tedious and error-prone. Common mistakes include:

- Ignoring oxygen atoms in sulfate or nitrate ions.
- Failing to conserve atoms when multiple products contain the same element (e.g., K in $\text{K}_2\text{Cr}_2\text{O}_7$ and K_2SO_4)
- Skipping hidden charges in species like Cr^{3+} or NO

MAPLE minimizes these issues by enabling users to:

- Formulate symbolic systems of elemental balances.
- Automatically solve for unknown coefficients.
- Normalize fractional results to integers.

In Example 5 (ethanol oxidation), MAPLE ensured conservation across C, H, O, Cr, K, and S—even with

sulfate groups appearing in several compounds. In Example 4 (ferrocyanide reaction), it managed more than seven element types and avoided mistakes common in manual algebraic balancing.

In educational settings, MAPLE not only prevents mistakes but also reinforces students' understanding of chemical conservation principles. In research or industrial contexts, it ensures reliable input for stoichiometric calculations, simulations, or yield analysis.

By integrating symbolic algebra and constraint solving, MAPLE acts as a powerful ally for anyone performing quantitative chemical reaction analysis.

7. Conclusion

This paper presented a structured approach for balancing chemical equations—ranging from simple redox systems to complex polyatomic reactions—using MAPLE software and linear algebra techniques. Manual balancing, while foundational for learning, quickly becomes unwieldy when faced with multiple elements, nested ions, or redox pairs. The integration of symbolic algebra in MAPLE enables chemists and educators to systematically solve and verify stoichiometric relationships while minimizing computational error.

By working through five diverse examples, this study demonstrated the versatility of MAPLE's symbolic engine. The software enabled fractional scaling, integer normalization, matrix manipulation, and even Gauss-Jordan reduction—all while maintaining chemical validity and logical transparency. Notably, MAPLE was particularly effective in handling large systems involving sulfate compounds, organic oxidation, and multiple oxidation states.

For instructors, this tool supports curriculum goals in general and analytical chemistry, allowing students to shift focus from repetitive arithmetic to conceptual learning. For researchers and professionals, it provides reliable workflows for automation, simulation input, and reaction pathway exploration.

Future studies may incorporate MAPLE's graphical capabilities or its integration with other symbolic engines like MATLAB or Python-SymPy. Additionally, hybrid approaches combining AI-assisted balancing with symbolic algebra could further enhance usability in educational and industrial contexts. Extensions could also include ionic charge balancing, pH-adjusted systems, and reaction yield modeling.

8. References

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