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A Localized Linear Substitution Algorithm for Balancing Complex Chemical Systems: Efficiency and Computational Complexity of the EFN Method

Nizami Rzayev*

Azerbaijan State Oil and Industry University (ASOIU), Computer Engineering Department, Baku, Azerbaijan

nrzayev971@gmail.com

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Abstract

Balancing complex chemical equations, particularly high-order redox reactions, is a fundamental yet computationally demanding task in chemistry. Conventional techniques, such as the standard algebraic method and the ion-electron method, often lead to overwhelming systems of linear equations or tedious multi-step procedures that are prone to human error. This paper proposes the EFN (Efficiency-Focused Normalization) method, a streamlined algorithmic approach designed to optimize the balancing process. While the EFN method shares its foundation with the classical algebraic method, it significantly diverges by employing a selective variable assignment strategy that reduces the number of unknowns. By prioritizing key elements and using localized substitution, the EFN method minimizes mathematical complexity and accelerates the solving process, making it possible to balance highly intricate equations within minutes. The efficiency of the proposed method is validated through several complex case studies, highlighting its po-

*Corresponding author.

tential for both educational purposes and computational chemistry applications.

1 Introduction

Balancing chemical equations is a fundamental process in academic research and industrial-scale stoichiometric calculations. This process, based on the law of conservation of mass, ensures the atomic balance between reactants and products. While traditional methods—particularly the classical algebraic and ion-electron methods—are effective for simple reactions, they pose significant time-consuming challenges and mathematical complexities when dealing with intricate redox equations [1,2]. Recent advancements in the field have explored diverse mathematical frameworks, including the application of Hilbert basis for achieving stoichiometric balance [4]. While traditional algebraic approaches and educational methods provide a solid basis for stoichiometry, they often lead to high computational complexity and variable redundancy in high-order complex systems.

This paper introduces the EFN (Efficiency-Focused Normalization) method, which aims to solve the computational load issues. Conceptually inspired by the "Everything from Nothing" principle, this algorithm allows for the derivation of the entire stoichiometric system using only one or two initial variables [3].

2 Methodology

The Efficiency-Focused Normalization (EFN) method is a systematic algorithmic approach designed to resolve chemical equations by minimizing the number of simultaneous equations. Unlike the standard algebraic method, which often requires solving a large matrix of variables, EFN identifies "anchor" compounds to establish a chain of linear dependencies.

The algorithm follows a structured four-phase process:

Phase I: Stoichiometric Mapping

The process initiates with the construction of a Distribution Table. Each reactant and product is treated as a distinct entity. The frequency of

every atomic element is recorded to identify elements that appear in the fewest number of compounds. These "low-frequency" elements serve as the starting points for the balancing process to ensure minimal variable propagation.

Phase II: Primary Variable Anchoring

A primary variable, designated as "X", is assigned to the most complex molecular species (the anchor). The coefficients of all constituent elements of this anchor are then immediately projected onto the opposite side of the equation. This creates a direct functional link between the reactant and product sides, effectively "locking" the ratios of several compounds simultaneously.

Phase III: Recursive Localized Substitution

For elements that appear in multiple compounds, secondary variables (e.g., "Y", "Z") are introduced only when necessary. Instead of solving a global system, EFN uses Localized Mass Balance Equations. Each element is balanced sequentially, expressing each new variable as a function of the previous ones. This recursive substitution reduces the complexity of the final mathematical expression.

Phase IV: Global Normalization and Integer Conversion

Once all species are expressed in terms of the primary variable "X" (or its derivatives), the system is normalized. If fractional coefficients exist, the entire equation is multiplied by the least common multiple (LCM) of the denominators to achieve the simplest whole-number ratio, fulfilling the law of conservation of mass.

3 "EFN method": Case study 1

$$Al + NH_4ClO_4 \rightarrow Al_2O_3 + AlCl_3 + NO + H_2O$$

1) Each entity is treated as a distinct chemical compound. A stoichiometric distribution table is then constructed:

Elements	Left side	Right side
Al	1	2
N	1	1
H	1	1
Cl	1	1
O	1	3

2) Since the elements “N”, “H”, and “Cl” appear in only one compound on both sides, the balancing process initiates with them. Given that each of these elements is contained within the NH_4ClO_4 molecule, the coefficient X is assigned to this compound.

$$Al + XNH_4ClO_4 \rightarrow Al_2O_3 + \frac{X}{3}AlCl_3 + XNO + 2XH_2O$$

3) The coefficient for Al_2O_3 is determined based on the balance of “O” atoms. By assuming the coefficient of Al_2O_3 as Y, the following equation is derived: $4X = 3Y + X + 2X \Rightarrow Y = X/3$. The Y is replaced by X/3:

$$Al + XNH_4ClO_4 \rightarrow \frac{X}{3}Al_2O_3 + \frac{X}{3}AlCl_3 + XNO + 2XH_2O$$

4) The coefficient for the “Al” reagent is determined based on the balance of “Al” atoms. By assuming the coefficient of “Al” as Z, the following equation is derived: $Z = 2(X/3) + X/3 = X$. The Z is replaced by X:

$$XAl + XNH_4ClO_4 \rightarrow \frac{X}{3}Al_2O_3 + \frac{X}{3}AlCl_3 + XNO + 2XH_2O$$

5) All coefficients are multiplied by 3 to achieve the simplest integer ratio:

$$3Al + 3NH_4ClO_4 \rightarrow Al_2O_3 + AlCl_3 + 3NO + 6H_2O \quad (1)$$

4 Case study 2: complex redox reaction

$$K_4Fe(SCN)_6 + K_2Cr_2O_7 + H_2SO_4 \rightarrow$$
$$Fe_2(SO_4)_3 + Cr_2(SO_4)_3 + CO_2 + H_2O + K_2SO_4 + KNO_3$$

1) A stoichiometric distribution table is constructed to specify the number of compounds containing each particular element on both the left (reactant) and right (product) sides of the equation.

Elements	Left side	Right side
K	2	2
Fe	1	1
S	2	3
C	1	1
N	1	1
Cr	1	1
O	2	6
H	1	1

2) Since the elements "Fe", "C", "N", "Cr", and "H" appear in only one compound on both sides of the equation, the balancing process initiates with these specific elements. Given that the majority of these elements are contained within the "$K_4Fe(SCN)_6$" molecule, the coefficient "X" is assigned to this compound, and the corresponding coefficients on the product (right) side are placed accordingly. Since only "Cr" and "H" among the listed elements remain without coefficients, the variable "Y" is assigned to "$K_2Cr_2O_7$" and "$Cr_2(SO_4)_3$", while the variable "Z" is assigned to the "H_2SO_4" and "H_2O" compounds.

$$X K_4Fe(SCN)_6 + Y K_2Cr_2O_7 + Z H_2SO_4 \rightarrow$$
$$\frac{X}{2} Fe_2(SO_4)_3 + Y Cr_2(SO_4)_3 + 6X CO_2 + Z H_2O + K_2SO_4 + 6X KNO_3$$

3) Subsequently, the remaining unused elements from the distribution table are identified, and their molar balances are verified sequentially, starting from the least frequent element. Among these, the element "K" is addressed first due to its lower frequency on both sides of the equation. Since only the "K_2SO_4" compound remains without a coefficient, a temporary variable "a" is assigned to it; this "a" coefficient is then substituted and expressed in terms of the other existing variables.

$$4X + 2Y = 2a + 6X \implies a = Y - X$$

$$X K_4Fe(SCN)_6 + Y K_2Cr_2O_7 + Z H_2SO_4 \rightarrow$$
$$\frac{X}{2} Fe_2(SO_4)_3 + Y Cr_2(SO_4)_3 + 6X CO_2 + Z H_2O + (Y - X) K_2SO_4 + 6X KNO_3$$

4) Following the same procedure, the molar balance of the element "S" is verified, and the coefficient "Z" is subsequently substituted and expressed in terms of the other primary variables.

$$6X + Z = \frac{3X}{2} + 3Y + (Y - X) \implies Z = 4Y - \frac{11X}{2}$$

$$X K_4Fe(SCN)_6 + Y K_2Cr_2O_7 + (4Y - \frac{11X}{2}) H_2SO_4 \rightarrow$$
$$\frac{X}{2} Fe_2(SO_4)_3 + Y Cr_2(SO_4)_3 + 6X CO_2 + (4Y - \frac{11X}{2}) H_2O$$
$$+ (Y - X) K_2SO_4 + 6X KNO_3$$

5) At this stage, only the element "O" remains in the distribution table. Therefore, by verifying its molar balance, all "Y" coefficients in the equation are substituted and expressed in terms of the "X" coefficients:

$$7Y + 4(4Y - \frac{11X}{2}) = 6X + 12Y + 12X + (4Y - \frac{11X}{2}) + 4(Y - X) + 18X$$
$$Y = \frac{97X}{6}$$

6) To eliminate the fractional coefficients, all values are multiplied by 6, and the variable "x" is factored out to achieve the final integer balance.

$$6K_4Fe(SCN)_6 + 97K_2Cr_2O_7 + 355H_2SO_4 \rightarrow$$
$$3Fe_2(SO_4)_3 + 97Cr_2(SO_4)_3 + 36CO_2 + 355H_2O + 91K_2SO_4 + 36KNO_3 \quad (2)$$

The balancing process is now complete. This methodology demon-

strates that regardless of the equation's complexity, a systematic solution can be achieved with relative ease. Consequently, this approach proves to be more time-efficient and reliable for solving high-order, complex chemical equations.

5 Comparative analysis

Table 1. Benchmarking of EFN against traditional methods

Feature	**Algebraic Method**	**Ion-Electron Method**	**EFN Method**
Math Load	High	Moderate	Low
Step Count	High	Moderate	Minimized
Error Proneness	High	Moderate	Low
Computational Ease	Complex	Difficult	Ideal

6 Conclusion

This article introduces a novel approach for balancing chemical equations, designated as the "EFN method". Compared to existing techniques, the EFN method is built upon simpler and more rapid computational logic. It provides significant time efficiency, particularly for high-order complex equations, by implementing a systematic mathematical framework for stoichiometric balancing.

Future automation and software integration of this method will further simplify chemical equation balancing in both educational and research environments. The algorithmic nature of the EFN method holds the potential for broad application across chemical engineering, analytical chemistry, and various industrial sectors. This research proposes a more efficient paradigm for regulating chemical reactions and establishes a foundational basis for future investigations in the field.

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