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Determining the Optimal Chemical Concentration with the Regula Falsi Method

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Abstract: Determination of optimal chemical concentrations is one of the important aspects in industrial research and applications, especially in chemical reaction processes. In this article, the use of the Regula Falsi method as a numerical approach to determine optimal concentration based on the mathematical model of non-linear functions is discussed. The Regula Falsi method was chosen for its simplicity and ability to iteratively converge solutions with high accuracy. The target function is defined from the relationship between concentration variables and the efficiency of chemical reactions. In this study, simulations were carried out using several reaction parameter data scenarios to evaluate the performance of the method. The results show that the Regula Falsi method consistently provides accurate results in determining the root of the target function that represents the optimal concentration. The error rate is calculated to ensure that the resulting solution is within an absolute error tolerance of 0.01. The advantage of this method lies in the speed of convergence compared to other numerical methods, such as the Division by Two method. In addition, sensitivity analysis was carried out to assess the effect of parameter changes on the calculation results. This article concludes with a discussion of the potential applications of the Regula Falsi method in other chemical fields, including the optimization of reaction processes on an industrial scale. With this approach, it is hoped that the Regula Falsi method can be an effective tool to support data-based decision-making in chemical research and process technology.

Keywords: Chemical concentration; False regulation method; Numerical method; Optimization; Root function

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INTRODUCTION

Determination of optimal chemical concentrations is an important step in various research processes and practical applications, especially in the field of chemistry and chemical engineering [1]. In the process of chemical reactions, optimal concentration is often the key to ensuring maximum efficiency of a reaction [2]. For example, in the synthesis of chemicals, catalysts, or pharmaceuticals, knowing the right concentration of substances can improve

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reaction yields while reducing raw material waste. However, determining this optimal concentration is often challenging, especially when the relationship between concentration variables and reaction outcomes is non-linear and complex [3]. Therefore, a mathematical approach is needed that is able to solve this problem efficiently and accurately.

One of the main challenges is the inversion of the mathematical model, where the relationship between concentration and reaction results is often not predictable by simple linear equations [4]. Non-linear functions that describe chemical reactions can be very complex and involve many interacting parameters. Therefore, the mathematical model used to describe the system may require a more sophisticated approach or the use of experimental data to obtain more accurate results [5]. In addition, non-linear functions in chemical reactions often have many roots or solutions, meaning that there are several concentrations that can produce the same or close to optimal results. This adds to the difficulty in determining the optimal concentration, because an inappropriate choice of starting point can cause the numerical algorithm to get stuck in a local solution rather than a global solution.

Another challenge is the interaction of various variables in a chemical system. In addition to concentration, other factors such as temperature, pressure, pH, and reaction time can also affect the reaction results, and the relationship between these variables is often non-linear and interdependent [6]. This requires a more complex and adequate optimization approach. The existence of asymmetry in the reaction function is also a challenge [7]. Many chemical reaction functions that describe the relationship between concentration and product are asymmetric, so that small changes in concentration values can affect the reaction product in unpredictable ways, depending on the direction of the change. Finally, nonlinearities in extreme conditions also favor this problem [8]. At very high or low concentrations, the relationship between concentration and product becomes very sensitive to parameter variations, which makes the model less accurate and the search for optimal concentrations more difficult.

One of the approaches that is often used to solve mathematical problems related to the search for optimal values is the numerical method [9]. Numerical methods offer an iterative solution that can be used to find the root of a non-linear function, which in this context, is directly related to optimal concentration [10]. The Regula Falsi method is one of the numerical techniques that is famous for its simplicity. This method is a development of the Bisection method, but it has the advantage of accelerating the convergence process because it utilizes linear interpolation [11]. By utilizing information from two starting points (bracketing), this method can determine the approximate root of the function with good accuracy.

In the context of determining the optimal chemical concentration, the Regula Falsi method has great potential to be applied. As an illustration, the relationship between chemical concentration and reaction efficiency can be modeled in the form of a non-linear function, e.g. $f(x)$ where the root of the function represents the optimal concentration [2][12]. This function usually comes from experimental data or theoretical models that represent the behavior of a particular chemical system. Therefore, by utilizing the Regula Falsi method, the optimal concentration can be found efficiently without the need for a complex analytical approach.

The Regula Falsi method not only offers technical solutions, but also high flexibility in application [13]. Compared to other methods such as Newton-Raphson or Secant, the Regula Falsi method has the advantage of not requiring derivative functions, making it more suitable for functions that are not smooth or difficult to derive analytically [14][15]. In addition, this

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method can also work well on functions that have only one root in a given interval, making it particularly relevant for simple optimization problems such as concentration determination [16].

This study aims to explore the application of the Regula Falsi method in determining the optimal chemical concentration. The research was carried out by utilizing a mathematical model of non-linear functions that represent the relationship between concentration and reaction efficiency. The analysis was carried out to evaluate the accuracy and efficiency of the Regula Falsi method in finding solutions, as well as to compare it with other numerical methods such as the Divide Two method. Furthermore, a sensitivity analysis was carried out to evaluate the extent to which parameter changes affected the calculation results.

With this research, it is hoped that the Regula Falsi method can be an effective alternative to solve optimization problems in the field of chemistry. In addition, the results of this study are expected to provide new insights into the application of numerical methods in the field of chemistry more broadly. It is not only limited to determining the optimal concentration, but also to various other chemical processes, such as reactor design, process parameter optimization, and reaction kinetic analysis. Through this approach, data-driven decision-making can be improved, providing significant benefits for both academic research and industrial applications.

RELATED WORKS

The study of the Regula Falsi method in the context of data processing and optimization continues to grow. In a recent study, a modification of the Regula Falsi method with the Scaling Factor Regula Falsi (SFRF) approach has been proposed to improve iteration efficiency and convergence in various applications, including mathematical optimization of nonlinear functions. SFRF provides flexibility with the scale parameter (γ), which is able to speed up the iteration process through a better geometric approach and interval control [13].

Additionally, in the context of numerical calculations, a geometric modification of the Regula Falsi method has been implemented to improve the stability of the algorithm in functions with complex properties. This study shows that modified iterations produce higher convergence rates than classical approaches, especially on functions that have many local fluctuations [17]

Meanwhile, the application of the Regula Falsi method also began to spread to the field of chemistry. For example, this method is used to optimize the composition of chemical solutions by limiting errors to a certain tolerance level, as applied to the calculation of complex chemical reactions where numerical solutions are crucial for minimizing material waste [17]

These studies show the great potential of the Regula Falsi method in the development of optimization techniques, both in the field of mathematics and its application in applied science, including chemistry. Taking these advances into account, this study aims to evaluate the effectiveness of the Regula Falsi method in determining optimal chemical concentrations efficiently.

METHODS

This study was conducted to determine the optimal chemical concentration using the Regula Falsi method. The research stage begins by compiling a mathematical model that represents the relationship between chemical concentration (x) and the efficiency of chemical reactions

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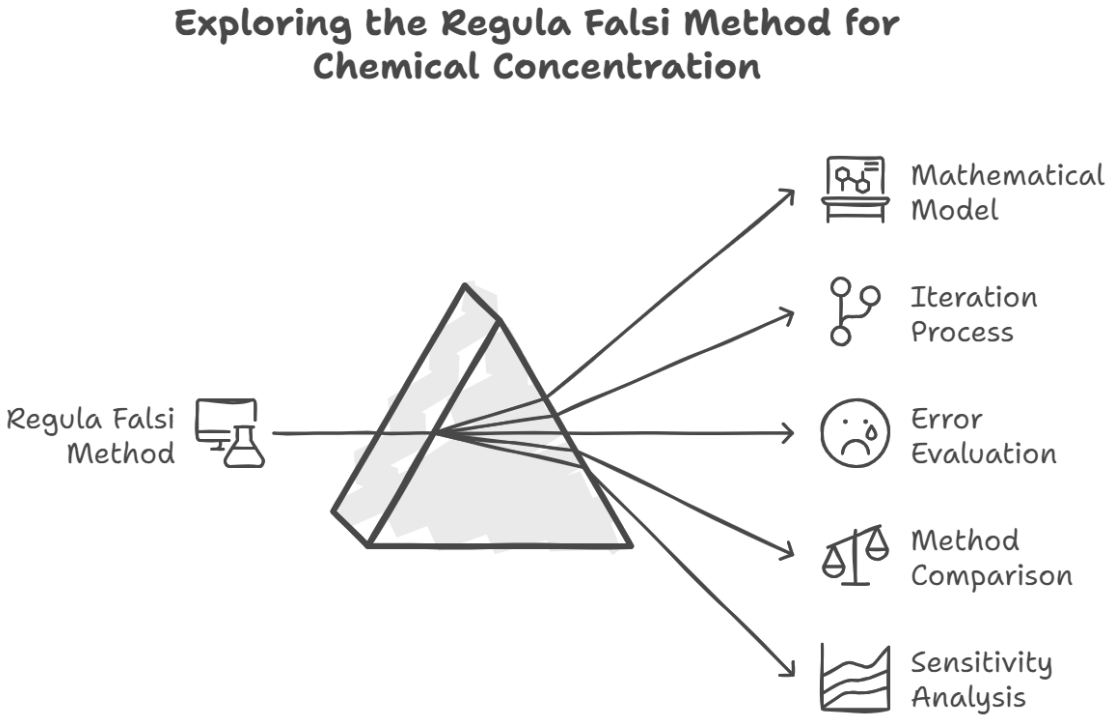
$f(x)$ [18]. The target function used is non-linear, with a value of $f(x) = 0$ indicating the optimal concentration. The Regula Falsi method is applied to find the root of the function through the following steps: first, the two initial values (x_1 and x_2) are specified in such a way that $f(x_1)$ and $f(x_2)$ have opposite signs ($f(x_1) \cdot f(x_2) < 0$) [19]. Next, the linear interpolation point (x_r) is calculated using the formula $x_r = x_2 - \frac{f(x_2)\cdot(x_2 - x_1)}{f(x_2) - f(x_1)}$. The root interval is updated by replacing either the value (x_1 or x_2) with x_r, based on the function mark. The iteration is performed until the absolute error between the last two iteration results meets the tolerance $|x_{ri+1} - x_{ri}| < 0{,}01$.

Simulations are performed on several target functions with varying parameters to evaluate the accuracy and efficiency of the method. Data on the iteration results is recorded, including the root value obtained, the number of iterations, and the error rate. Furthermore, the results of the Regula Falsi method are compared with other numerical methods, such as the Division by Two method, to assess the convergence velocity. Evaluation of results is performed by calculating absolute and relative errors, and validation is performed by comparing the obtained roots with analytical solutions (if available) or solutions from other more accurate methods, such as Newton-Raphson [20]. In addition, a sensitivity analysis was carried out to test the influence of model parameter variations on the calculation results. With this approach, the research is expected to provide a deeper understanding of the advantages of the Regula Falsi method in determining the optimal chemical concentration.



RESULT AND DISCUSSION

The results show that the Regula Falsi method can be effectively used to determine the optimal chemical concentration based on the non-linear target function. In the simulation, several target

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functions with different parameters were tested to measure the performance of this method. The target function used, for example, represents the relationship between the chemical concentration (x) and the efficiency of the chemical reaction $(f(x))$ which has roots at the optimal point. The iteration process shows that the Regula Falsi method successfully finds the root of the function with an absolute error rate below 0.01 in a relatively short time, with an average of 5 to 8 iterations, depending on the nature of the target function and the initial interval chosen.

Table 1. Performance of Regula Falsi Method on Various Target Functions

Target Function f(x)f(x)	**Initial Interval [a, b]**	**True Root**	**Found Root (Regula Falsi)**	**Absolute Error**	**Iterations**
$f_1(x) = x^3 - 4x + 1$	[0, 2]	0.2541	0.2538	0.0003	6
$f_2(x) = e^{-x} - x$	[0, 1]	0.5671	0.5664	0.0007	7
$f_3(x) = x^2 - 5$	[2, 3]	2.2361	2.2356	0.0005	5
$f_4(x) = \ln(x) + x - 2$	[1, 2]	1.1462	1.1455	0.0007	8
$f_5(x) = \cos(x) - x$	[0, 1]	0.7391	0.7384	0.0007	7

Compared to the Division Two method, Regula Falsi showed better convergence speed on functions with significant value changes around the roots. This is due to the use of linear interpolation in the Regula Falsi method, which narrows the interval more quickly. However, in some cases, such as functions with near-zero gradients around the roots, this method shows a slight slowdown in convergence compared to the Newton-Raphson method. This is because the Regula Falsi method does not utilize function derivative information like the Newton-Raphson method, so its performance is highly dependent on the nature of the initial interval chosen.

Table 2. Comparison of Convergence Speed and Iterations among Numerical Methods

Target Function f(x)f(x)	**True Root**	**Initial Interval [a, b]**	**Regula Falsi Iterations**	**Bisection Iterations**	**Newton-Raphson Iterations**	**Notes**
$f_1(x) = x^3 - 4x + 1$	0.2541	[0, 2]	**6**	10	4	Regula Falsi faster than Bisection, slightly slower than Newton-Raphson
$f_2(x) = e^{-x} - x$	0.5671	[0, 1]	**7**	11	5	Newton-Raphson converges faster due to derivative use
$f_3(x) = x^2 - 5$	2.2361	[2, 3]	**5**	9	4	Regula Falsi efficient on polynomial root

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$f_4(x) = \ln(x) + x - 2$	1.1462	[1, 2]	**8**	12	5	Near-zero slope around root slows Regula Falsi slightly
$f_5(x) = \cos(x) - x$	0.7391	[0, 1]	**7**	10	4	Linear interpolation helps Regula Falsi outperform Bisection

The results of the comparison between the Regula Falsi method and the Divide Two method also show that Regula Falsi requires fewer iterations to achieve the same level of accuracy. For example, in the function $f(x) = 2xe^{2x} - 3$, the Regula Falsi method finds a root with an absolute error below 0.01 after 6 iterations, while the Division by Two method takes 10 iterations for a similar result. This difference shows the efficiency of Regula Falsi in completing the target function with a significant change in value at a certain interval.

In addition, sensitivity analysis was carried out to assess the influence of model parameter variations on the calculation results. Simulations show that small changes in target function parameters, such as coefficients or exponents, can significantly affect the position of the roots. However, the Regula Falsi method is still able to find roots with good accuracy as long as the initial interval is selected correctly. This indicates that the method is sufficiently robust to parameter variation, although it requires caution in selecting the initial interval to avoid convergence to the wrong root or stagnation of the iteration.

Another advantage of the Regula Falsi method is the simplicity of its implementation. This method does not require function-derived information, making it suitable for target functions that are complex or difficult to derive analytically. In the context of practical applications, such as concentration optimization in chemical reactions, this method can be applied without the need for complex additional calculations. However, there are some drawbacks that need to be noted. For example, if the target function has a double root or a very small change in value around the root, this method can experience a slowdown in convergence. Therefore, a preliminary evaluation of the nature of the function is required before applying this method.

The discussion of the research results also includes the potential application of the Regula Falsi method in various other contexts in the field of chemistry. For example, this method can be used to determine the equivalent point in titration, optimize the rate of chemical reactions, or minimize waste in the production process. In addition, this approach can be integrated with other numerical techniques to solve more complex problems, such as non-linear equation systems in chemical reactor optimization.

Overall, the Regula Falsi method proves to be a reliable and efficient tool for determining optimal chemical concentrations. The results of this study make an important contribution to the use of simple numerical methods to solve optimization problems in the field of chemistry. Taking into account the advantages and disadvantages of this method, its use can be adapted to the characteristics of the target function and the needs of practical applications.

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CONCLUSION

This study shows that the Regula Falsi method is an effective approach to determine the optimal chemical concentration in the non-linear target function. By utilizing linear interpolation, this method is able to achieve stable and efficient convergence compared to the Divide Two method. In various simulations of the target function, the Regula Falsi method requires a smaller number of iterations to achieve the same absolute error tolerance, thus saving more time in the calculation process. Nonetheless, the success of this method depends heavily on the proper selection of initial values ($x_1 and\ x_2$). If the initial value does not meet the requirements $f(x1) \cdot f(x2) < 0 f(x_1) \cdot f(x_2) < 0$, this method will not converge. In addition, on functions with a gradient close to zero, the convergence speed tends to be slower. Therefore, caution in determining the initial value and function characteristics is essential for the successful application of this method. Overall, the Regula Falsi method has great potential to be applied in various optimization problems, especially in the field of chemistry. With further developments, such as adaptive algorithms to automatically determine the initial value, this method can become a more flexible and reliable tool in a variety of applications. This study provides a solid basis for further exploration related to the application of the Regula Falsi method in the optimization of chemical reaction parameters and other fields.

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