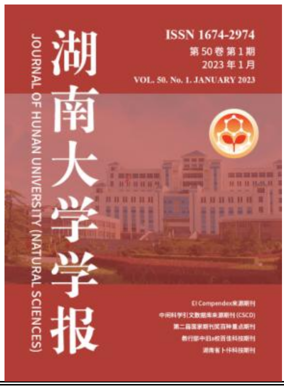

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Solution of Chemical Engineering Models and Their Dynamics Using a New Three-Step Derivative Free Optimal Method

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Abstract: The aim of this research article is to develop a three-step optimal iterative technique using Hermite interpolation for the solution of nonlinear algebraic and transcendental equation arises in chemical engineering models. In this connection, we proposed an optimal three-step eight-order technique without derivative and, has a high efficiency index. The convergence analysis of the proposed method is also discussed. For this demonstration, we apply the new technique to certain nonlinear problems in chemical engineering, such as, the conversion in a chemical reactor, a chemical equilibrium problem, azeotropic point of a binary solution and Continuous Stirred Tank Reactor (CSTR). And the study of dynamics is also used to demonstrate the performance of the presented scheme. It's observed from the Comparison tables and dynamics, the proposed technique is more efficient compared to other existing methods.

Keywords: nonlinear equations, root-finding iterative methods, chemical engineering models, optimal order of convergence, basin of attraction.

使用新的三步无导数优化方法求解化学工程模型及其动力学

摘要：本研究文章的目的是开发一种使用埃尔米特插值的三步最优迭代技术，用于求解化学工程模型中出现的非线性代数和超越方程。在此方面，我们提出了一种最优的三步八阶技术，无需导数，具有很高的效率指标。还讨论了所提出方法的收敛性分析。在本次演示中，我们将新技术应用于化学工程中的某些非线性问题，例如化学反应器中的转化、化学平衡问题、二元溶液的共沸点和连续搅拌釜反应器(CSTR)。并且动力学研究也用于证明所提出方案的性能。从比较表和动力学观察，与其他现有方法相比，所提出的技术更有效。

关键词：非线性方程，寻根迭代法，化学工程模型，收敛的最佳顺序，吸引盆地。

1. Introduction

Determining the solution of 0, when is nonlinear, is of high concern in both applied and real-life models. In this article, the proposed method will be tested by models in chemical engineering, i.e., conversion in a chemical reactor, a chemical equilibrium problem, azeotropic point of a binary solution and Continuous Stirred Tank Reactor (CSTR).

In this regard, the Newton Raphson technique for solving such equations already exists

$$\mu_{n+1} = \mu_n - \frac{\zeta(\mu_n)}{\zeta'(\mu_n)} \tag{1}$$

Equation 1 is one of the most well-known and renowned iterative approaches for finding solutions to nonlinear equation is the Newton Raphson method [1]. However, Newton's method has a quadratic convergence and requires two function evaluations, i.e., $\zeta(\mu)$ & $\zeta'(\mu)$, if $\zeta'(\mu) = 0$; then, the said method fails to converge. The methods involve derivative required more computing cost compared to methods with derivative requirements. Nowadays scholars more intend to derivative free methods.

Steffensen developed a derivative-free iterative method [2]–[4].

$$\psi_n = \mu_n + \zeta(\mu_n), \qquad \mu_{n+1} = \mu_n - \frac{\zeta(\mu_n)}{\zeta[\mu_n, \psi_n]} \tag{2}$$

where $[\mu_n, \psi_n] = \frac{\zeta(\mu_n) - \zeta(\psi_n)}{\mu_n - \psi_n}$, it maintains the same convergence order and efficiency index as Newton's method. For an optimal convergence order $2^{\rho-1}$ [2], where ρ functional evaluations per iteration.

A three-step technique of eighth order of convergence with four-function evaluation was proposed in [5]. It is denoted by "SM", i.e.,

$$\left.\begin{array}{l}
\text{Step 1. } v_n = \mu_n - \frac{\zeta(\mu_n)}{\zeta[\mu_n, \psi_n]}, \quad \text{where } \psi_n = \zeta(\mu_n + \zeta(\mu_n)) \\
\text{Step 2. } \xi_n = v_n - \frac{\zeta(v_n)}{\left(\zeta[\mu_n, \psi_n]\left(1 - \frac{\zeta(v_n)}{\zeta(\mu_n)} - \frac{\zeta(v_n)}{\zeta(\psi_n)}\right)\right)} \\
\text{Step 3. } \mu_{n+1} = \left(\xi_n - \frac{\zeta(\xi_n)}{\zeta[\mu_n, \psi_n]} \frac{a}{\left(1 - \frac{\zeta(v_n)}{\zeta(\mu_n)} - \frac{\zeta(v_n)}{\zeta(\psi_n)}\right)}\right), \quad \text{where} \\
a = \left(\begin{array}{c}
1 + \frac{\left(\frac{\zeta(v_n)}{\zeta(\mu_n)}\right)^2}{1 + \zeta[\mu_n, \psi_n]} + \\
(1 + \zeta[\mu_n, \psi_n])(2 + \zeta[\mu_n, \psi_n])\left(\frac{\zeta(v_n)}{\zeta(\psi_n)}\right)^3 + \frac{\zeta(\xi_n)}{\zeta(v_n)} \\
+ \left(\frac{\zeta(\xi_n)}{\zeta(v_n)}\right)^2 + \frac{\zeta(\xi_n)}{\zeta(\mu_n)} + \frac{\zeta(\xi_n)}{\zeta(\psi_n)}
\end{array}\right)
\end{array}\right\} \tag{3}$$

The Chebyshev-Halley type derivative free method for numerical solution of nonlinear equations of eighth order was presented in [6]. It required four-function evaluation and solved some real-life problems in different fields denoted by "AKKB".

$$\left.\begin{array}{l}
\text{Step 1. } v_n = \mu_n - \frac{\zeta(\mu_n)}{\zeta[\mu_n, \psi_n]}, \text{where } \psi_n = \zeta(\mu_n + \zeta(\mu_n)) \\
\text{Step 2. } \xi_n = \zeta(v_n) - \left[\frac{\zeta(v_n)}{\zeta(\mu_n) - 2\zeta(v_n)} \cdot \frac{\zeta(\mu_n)}{\zeta[v_n, \psi_n]}\right]\left(\frac{1}{1 + \frac{\zeta(v_n)}{\zeta(v_n)}}\right) \\
\text{Step 3. } \mu_{n+1} = \left(\xi_n - \frac{\zeta(\xi_n)}{\zeta[\xi_n, v_n] + (\xi_n - v_n)\zeta[\xi_n, v_n, \mu_n] + (\xi_n - v_n)(\xi_n - \mu_n)\zeta[\xi_n, v_n, \mu_n, \psi_n]}\right)
\end{array}\right\} \tag{4}$$

An eighth-order derivative free iterative method for the solution of nonlinear equations based on Steffensen-King's type methods was presented in [7]. It required four-function evaluation per iteration, denoted by "KBK".

$$\left.\begin{array}{l}
\text{Step 1. } v_n = \mu_n - \frac{\zeta(\mu_n)}{\zeta[\mu_n, \psi_n]}, \text{where } \psi_n = \zeta(\mu_n + \zeta^3(\mu_n)) \\
\text{Step 2. } \xi_n = v_n - \left[\frac{\zeta(v_n)}{2\zeta[v_n, \mu_n] - \zeta[\mu_n, \psi_n]}\right], \\
\text{Step 3. } \mu_{n+1} = \xi_n - \frac{\zeta(\xi_n)}{\zeta[v_n, \xi_n] + (\xi_n - v_n)\zeta[\psi_n, v_n, \xi_n]}\left\{1 - \left(\frac{\zeta(v_n)}{\zeta(\mu_n)}\right)^3\right. \\
\left. - \left(\frac{\zeta(v_n)}{\zeta(\mu_n)}\right)^3 - 8\frac{\zeta(v_n)\,\zeta(\xi_n)}{\zeta^2(\mu_n)} - \frac{\zeta(\xi_n)}{\zeta(\mu_n)} + 5\left(\frac{\zeta(\xi_n)}{\zeta(v_n)}\right)^2\right\}
\end{array}\right\} \tag{5}$$

An optimal eighth-order derivative free method was proposed in [8] based on the Steffensen-type method and they also study the dynamic behavior of the proposed method for demonstration; it is denoted by JLM.

$$\left.\begin{array}{l}
\text{Step 1. } v_n = \mu_n - \frac{\zeta(\mu_n)}{\zeta[\psi_n, \mu_n]}, \text{ where } \psi_n = \zeta(\mu_n + \zeta^3(\mu_n)) \\
\text{Step 2. } \xi_n = v_n - \left[\frac{\zeta(v_n)}{\zeta[v_n, \psi_n] - (v_n - \psi_n)\zeta[v_n, \psi_n, \mu_n]}\right], \\
\text{Step 3. } \mu_{n+1} = \xi_n - \frac{\zeta(\xi_n)}{\zeta[\xi_n, v_n] + (\xi_n - v_n)\zeta[\xi_n, v_n, \psi_n] + (\xi_n - v_n)(\xi_n - \psi_n)\zeta[\xi_n, v_n, \psi_n, \mu_n]}
\end{array}\right\} \tag{6}$$

Many scholars proposed iterative methods for various orders of convergence and efficiency indexes, and test these iterative methods in application problems of various fields, i.e., medical science: blood rheology, non-Newtonian mechanics, fluid dynamics, population dynamics, and neurophysiology, chemical engineering: conversion in a chemical reactor, a chemical equilibrium problem, azeotropic point of a binary solution and Continuous Stirred Tank Reactor (CSTR), physics, civil engineering, etc. [9]–[27].

2. Proposed Method

Recently, a non-optimal eighth-order method with five-function evaluation (three functions and two first derivative) was proposed in [28], i.e.,

$$\left.\begin{array}{l}
\text{Step 1. } v_n = \mu_n - \frac{\zeta(\mu_n)}{\zeta'(\mu_n)} \\
\text{Step 2. } \xi_n = v_n - \frac{\zeta(v_n)}{\zeta'(\mu_n)} \frac{\zeta^2(\mu_n)}{(\zeta^2(\mu_n) - 2\zeta(v_n)\zeta(\mu_n) + \zeta^2(v_n))} \\
\text{Step 3. } \mu_{n+1} = \xi_n - \frac{\zeta(\xi_n)}{\zeta'(\xi_n)}
\end{array}\right\} \tag{7}$$

In Equation 7, we have two derivatives $\zeta'(\mu_n)$ and $\zeta'(\xi_n)$. In connection of the derivative free method, we must replace these with derivatives $\zeta'(\mu_n) \approx \zeta[\mu_n, \psi_n]$ taken from equations (5) and (6).

We approximate $\zeta'(\xi_n)$ using available data. Since we have four values $\zeta(\mu), \zeta'(\mu), \zeta(v), \zeta(\xi)$ approximate ζ by its Hermite's interpolating polynomial H_3 of degree 3 at the nodes μ, v, ξ and use the approximation $\zeta'(\xi) \approx H_3'(\xi)$ in the third step of the iterative scheme (7)

Hermite's interpolating polynomial of third degree has the form

$$H_3(\rho) = \varsigma_0 + \varsigma_1(\rho - \mu) + \varsigma_2(\rho - \mu)^2 + \varsigma_3(\rho - \mu)^3 \tag{8}$$

and its derivative is

$$H_3'(\rho) = \varsigma_1 + 2\varsigma_2(\rho - \mu) + 3\varsigma_3(\rho - \mu)^2 \tag{9}$$

The unknown coefficients will be determined using available data from the conditions: $H_3(\mu) = \zeta(\mu)$, $(v) = \zeta(v), (\xi) = \zeta(\xi)$ and $H_3'(\mu) = \zeta'(\mu)$.

Putting $\rho = \mu$ into equation (8) and equation (9), we get $\varsigma_0 = \zeta(\mu)$ and $\varsigma_1 = \zeta'(\mu)$. The coefficients ς_2 and ς_3 are obtained from the system of two linear equations formed using the remaining two conditions $\rho = \nu \; and \; \rho = \xi$ in equation (8), and we obtain

$$\varsigma_2 = \frac{(\xi-\mu)\zeta[\nu,\mu]}{(\xi-\nu)(\nu-\mu)} - \frac{(\nu-\mu)\zeta[\xi,\mu]}{(\xi-\nu)(\xi-\mu)} - \zeta'(\mu)\left(\frac{1}{\xi-\mu} - \frac{1}{\nu-\mu}\right) \quad (10)$$

and

$$\varsigma_3 = \frac{\zeta[\xi,\mu]}{(\xi-\nu)(\xi-\mu)} - \frac{\zeta[\nu,\mu]}{(\xi-\nu)(\nu-\mu)} + \frac{\zeta'(\mu)}{(\xi-\mu)(\nu-\mu)} \quad (11)$$

By putting the values of $\varsigma_1, \varsigma_2, \varsigma_3$ & $\rho = \xi$ (9), we get

$$H_3'(z) = 2(\zeta[\mu,\xi] - \zeta[\mu.\nu]) + \zeta[\nu,\xi] + \frac{\nu-\xi}{\nu-\mu}\left(\zeta[\mu,\nu] - \zeta'(\mu)\right) \quad (12)$$

We replace $\zeta'(\xi_n)$ and $\zeta'(\mu_n)$ in equation (7), finally we obtain

$$\left.\begin{array}{l} \text{Step 1. } \nu_n = \mu_n - \frac{\zeta(\mu_n)}{\zeta[\psi_n,\mu_n]} \\ \text{Step 2. } \xi_n = \nu_n - \frac{\zeta(\nu_n)}{\zeta[\psi_n,\mu_n]} \frac{\zeta^2(\mu_n)}{(\zeta^2(\mu_n) - 2\zeta(\nu_n)\zeta(\mu_n) + \zeta^2(\nu_n))} \\ \text{Step 3. } \mu_{n+1} = \xi_n - \frac{\zeta(\xi_n)}{2(\zeta[\mu_n,\xi_n] - \zeta[\mu_n.\nu_n]) + \zeta[\nu_n,\xi_n] + \frac{\nu_n-\xi_n}{\nu_n-\mu_n}(\zeta[\mu_n,\nu_n] - \zeta[\psi_n,\mu_n])} \end{array}\right\} \quad (13)$$

According to [2] Equation (13) is an optimal, eighth-order derivative free method.

3. Convergence Analysis

Theorem: Let $\alpha \in D$ be a simple zero of a sufficiently differentiable function $\zeta : D \subset R \rightarrow R$ in an open interval D, which contains x_0 as an initial approximation of α. Then, the method (13) is of the eighth order and includes only four function evaluations per full iteration, and no derivatives used.

Proof: The Taylor's series expansion of the function $\zeta(\mu_n)$ can be written as:

$$\zeta(\mu_n) = \sum_{m=0}^{\infty} \frac{\zeta^m(\alpha)}{m!}(\mu_n - \alpha)^m = \zeta(\alpha) + \zeta'(\alpha)(\mu_n - \alpha) + \frac{\zeta''(\alpha)}{2!}(\mu_n-\alpha)^2 + \frac{\zeta'''(\alpha)}{3!}(\mu_n-\alpha)^3 + \cdots \quad (14)$$

For simplicity, we assume that $A_k = \left(\frac{1}{k!}\right)\frac{\zeta^k(\alpha)}{\zeta'(\alpha)}, k \geq 2,$ and assume that $e_n = \mu_n - \alpha$. Thus, we have

$$\zeta(\mu_n) = \zeta'(\alpha)[e_n + A_2 e_n{}^2 + A_3 e_n^3 + A_4 e_n^4 + \cdots] \quad (15)$$

Furthermore, we have

$$\zeta[\psi_n, \mu_n] = \frac{\zeta(\psi_n) - \zeta(\mu_n)}{\psi_n - \mu_n} = \zeta'(\alpha)\left(1 + 2A_2 e_n + 3A_3 e_n^2 + e_n^3\left(A_2\zeta'^3(\alpha) + 4A_4\right) + 3e_n^4\zeta'^3(\alpha)(A_2^2 + A_3) + 3e_n^5\zeta'^3(\alpha)(A_2^3 + 4A_2A_3 + 2A_4) + \cdots + O(e_n^9)\right) \quad (16)$$

$Step$ 1: $$\nu_n = \mu_n - \frac{\zeta(\mu_n)}{\zeta[\psi_n, \mu_n]} = A_2 e_n^2 - 2e_n^3(A_2^2 - A_3) + e_n^4\left(4A_2^3 - 7A_2A_3 + A_2\zeta'^3(\alpha) + 3A_4\right) + e_n^5\left(-8A_2^4 + 20A_2^2A_3 - 10A_2A_4 - 6A_3^2 + 3A_3\zeta'^3(\alpha)\right) + \cdots + O(e_n^9) \quad (17)$$

and

$$\zeta(\nu_n) = \zeta'(\alpha)\Big[A_2e_n^2 - 2e_n^3(A_2^2 - A_3) + e_n^4\left(4A_2^3 - 7A_2A_3 + A_2\zeta'^3(\alpha) + 3A_4\right) + e_n^5\left(-8A_2^4 + 20A_2^2A_3 - 10A_2A_4 - 6A_3^2 + 3A_3\zeta'^3(\alpha)\right) + \cdots + O(e_n^9)\Big] \quad (18)$$

From equations (16) and (18)

$$\frac{\zeta(\nu_n)}{\zeta[\psi_n, \mu_n]} = A_2e_n^2 - 2e_n^3(2A_2^2 - A_3) + e_n^4\left(13A_2^3 - 14A_2A_3 + A_2\zeta'^3(\alpha) + 3A_4\right) + e_n^5\left(-38A_2^4 + 64A_2^2A_3 - 3A_2^2\zeta'^3(\alpha) - 20A_2A_4 - 12A_3^2 + 3A_3\zeta'^3(\alpha)\right) + \cdots + O(e_n^9) \quad (19)$$

$$\zeta^2(\mu_n) - 2\zeta(\nu_n)\zeta(\mu_n) + \zeta^2(\nu_n) = e_n^2\zeta'^2(\alpha)\Big(1 + 2e_n^2(2A_2^2 - A_3) - 2e_n^3\left(5A_2^3 - 7A_2A_3 + A_2\zeta'^3(\alpha) + 2A_4\right) + \cdots\Big) \quad (20)$$

and

$$\frac{\zeta^2(\mu_n)}{\zeta^2(\mu_n) - 2\zeta(\nu_n)\zeta(\mu_n) + \zeta^2(\nu_n)} = 1 + 2A_2e_n + e_n^2(4A_3 - 3A_2^2) + 2e_n^3\left(A_2^3 - 4A_2A_3 + A_2\zeta'^3(\alpha) + 3A_4\right) + 2e_n^4\left(2A_2^4 + A_2^2A_3 + 2A_2^2\zeta'^3(\alpha) - 5A_2A_4 - 2A_3^2 + 3A_3\zeta'^3(\alpha)\right) + 2e_n^5\left(-9A_2^5 + 19A_2^3A_3 - A_2^3\zeta'^3(\alpha) - 5A_2A_3^2 + 9A_2A_3\zeta'^3(\alpha) - 4A_3A_4 + 6A_4\zeta'^3(\alpha)\right) + \cdots + O(e_n^9) \quad (21)$$

From equations (19) and (21), we have

$$\frac{\zeta(\nu_n)}{\zeta[\psi_n,\mu_n]}\left(\frac{\zeta^2(\mu_n)}{\zeta^2(\mu_n) - 2\zeta(\nu_n)\zeta(\mu_n) + \zeta^2(\nu_n)}\right) = A_2e_n^2 - 2e_n^3(A_2^2 - A_3) + e_n^4\left(2A_2^3 - 6A_2A_3 + A_2\zeta'^3(\alpha) + 3A_4\right) + e_n^5\left(2A_2^4 + 6A_2^2A_3 + A_2^2\zeta'^3(\alpha) - 8A_2A_4 - 4A_3^2 + 3A_3\zeta'^3(\alpha)\right) + \cdots + O(e_n^9) \quad (22)$$

and

Step 2:

$$\xi_n = \nu_n - \frac{\zeta(\nu_n)}{\zeta[\psi_n,\mu_n]}\left(\frac{\zeta^2(\mu_n)}{\zeta^2(\mu_n) - 2\zeta(\nu_n)\zeta(\mu_n) + \zeta^2(\nu_n)}\right) = e_n^4(2A_2^3 - A_2A_3) + e_n^5\left(-10A_2^4 + 14A_2^2A_3 - A_2^2\zeta'^3(\alpha) - 2A_2A_4 - 2A_3^2\right) + e_n^6\left(31A_2^5 - 72A_2^3A_3 + 4A_2^3\zeta'^3(\alpha) + 21A_2^2A_4 + 30A_2A_3^2 - 6A_2A_3\zeta'^3(\alpha) - 7A_3A_4\right) + \cdots + O(e_n^9) \quad (23)$$

$$\zeta(\xi_n) = \zeta'(\alpha)\left[e_n^4(2A_2^3 - A_2A_3) + e_n^5\left(-10A_2^4 + 14A_2^2A_3 - A_2^2\zeta'^3(\alpha) - 2A_2A_4 - 2A_3^2\right) + \cdots + O(e_n^9)\right] \quad (24)$$

$$\mu_{n+1} = \xi_n - \frac{\zeta(\xi_n)}{\zeta'(\xi_n)}, \text{ where } \zeta'(\xi_n) \approx H_3'(\xi_n)$$

$$H_3'(\xi_n) = 2(\zeta[\mu_n,\xi_n] - \zeta[\mu_n.\nu_n]) + \zeta[\nu_n,\xi_n] + \frac{\nu_n-\xi_n}{\nu_n-\mu_n}(\zeta[\mu_n,\nu_n] - \zeta[\psi_n,\mu_n]) \quad (25)$$

$$H'_3(\xi_n) = \zeta'(\alpha)\Big[1 + A_2e_n^4\left(4A_2^3 - 2A_2A_3 + A_2\zeta'^3(\alpha) + A_4\right) + e_n^5\left(-20A_2^5 + 28A_2^3A_3 - 6A_2^2A_4 - 4A_2A_3^2 + 5A_2A_3\zeta'^3(\alpha) + 2A_3A_4\right) + \cdots + O(e_n^9)\Big] \quad (26)$$

$$\frac{\zeta(\xi_n)}{H_3'(\xi_n)} = e_n^4(2A_2^3 - A_2A_3) + e_n^5\left(-10A_2^4 + 14A_2^2A_3 - A_2^2\zeta'^3(\alpha) - 2A_2A_4 - 2A_3^2\right) + \cdots + O(e_n^9) \quad (27)$$

Finally, we obtain

Step 3: $$\mu_{n+1} = \xi_n - \frac{\zeta(\xi_n)}{H_3'(\xi_n)} = A_2^2e_n^8(2A_2^2 - A3)(2A_2^3 - A_2A_3 + A_4) + O[e_n^9] \quad (28)$$

4. Numerical Experiment

The following problems are taken from the literature and tested by the proposed method.

Example 1 (conversion in a chemical reactor): See in [14], [29], [30], the following nonlinear equation is to be solved:

$$\zeta_1(\mu) = \frac{\mu}{1-\mu} - 5\log\left(\frac{0.4(1-\mu)}{0.4-0.5\mu}\right) + 4.45977 \quad (29)$$

As an initial solution, we selected $\mu_0 = 0.76$.

Table 1 Numerical results for Example 1 for the first four iterations and their absolute function values at $\mu_0 = 0.76$ (Developed by the authors)

Methods	Iteration	1st Iteration	2nd Iteration	3rd Iteration	4th Iteration
Proposed 8th	μ	7.57396×10^{-1}	7.57396×10^{-1}	7.57396×10^{-1}	7.57396×10^{-1}
	$\lvert\zeta(\mu)\rvert$	4.29446×10^{-9}	2.86660×10^{-72}	1.12989×10^{-577}	$6.58236 \times 10^{-4621}$
SM 8th	μ	7.57394×10^{-1}	7.57396×10^{-1}	7.57396×10^{-1}	7.57396×10^{-1}
	$\lvert\zeta(\mu)\rvert$	1.41787×10^{-4}	3.23556×10^{-28}	2.36985×10^{-217}	$1.96285 \times 10^{-1730}$
AKKB 8th	μ	7.59742×10^{-1}	7.59013×10^{-1}	7.57917×10^{-1}	7.57398×10^{-1}
	$\lvert\zeta(\mu)\rvert$	1.94304×10^{-1}	1.32320×10^{-1}	4.19134×10^{-2}	1.42725×10^{-4}
KBK 8th	μ	7.57399×10^{-1}	7.57396×10^{-1}	7.57396×10^{-1}	7.57396×10^{-1}
	$\lvert\zeta(\mu)\rvert$	1.93828×10^{-4}	1.15904×10^{-33}	4.39345×10^{-267}	$1.87274 \times 10^{-2134}$
JLM 8th	μ	7.57396×10^{-1}	7.57396×10^{-1}	7.57396×10^{-1}	7.57396×10^{-1}
	$\lvert\zeta(\mu)\rvert$	4.18512×10^{-7}	1.51627×10^{-42}	3.42909×10^{-255}	$4.58775 \times 10^{-1531}$

Table 2 Numerical results for Example 1, error fixed at $\delta = 10^{-3000}$ (Developed by the authors)

Methods	IG	N	FE	CPU Time
Proposed 8th	0.76	4	16	1.921
SM 8th	0.76	5	20	3.266
AKKB 8th	0.76	8	32	5.469
KBK 8th	0.76	5	20	3.625
JLM 8th	0.76	5	20	3.297

Example 2 (a chemical equilibrium problem) [13], [24], [26]:

$$\zeta_2(\mu) = \mu^4 - 7.79075\mu^3 + 14.7445\mu^2 + 2.511\mu - 1.674 \quad (30)$$

Table 3 Numerical results for Example 2 for the first four iterations and their absolute function values at $\mu_0 = 0.35$ (Developed by the authors)

Methods	Iteration	1st Iteration	2nd Iteration	3rd Iteration	4th Iteration
Proposed 8th	μ	2.77883×10^{-1}	2.77871×10^{-1}	2.77871×10^{-1}	2.77871×10^{-1}
	$\lvert\zeta(\mu)\rvert$	1.09725×10^{-4}	2.88117×10^{-38}	6.57149×10^{-307}	$4.81304 \times 10^{-2456}$
SM 8th	μ	2.77874×10^{-1}	2.77871×10^{-1}	2.77871×10^{-1}	2.00212×10^{-1}
	$\lvert\zeta(\mu)\rvert$	2.50859×10^{-5}	1.11091×10^{-38}	1.64358×10^{-305}	$3.77303 \times 10^{-2440}$
AKKB 8th	μ	2.77873×10^{-1}	2.77871×10^{-1}	2.77871×10^{-1}	2.77871×10^{-1}
	$\lvert\zeta(\mu)\rvert$	1.87514×10^{-5}	7.58534×10^{-39}	5.44010×10^{-306}	$3.80769 \times 10^{-2443}$
KBK 8th	μ	2.78568×10^{-1}	2.77871×10^{-1}	2.77871×10^{-1}	2.77871×10^{-1}
	$\lvert\zeta(\mu)\rvert$	6.26823×10^{-3}	3.93074×10^{-22}	1.33588×10^{-175}	$2.37747 \times 10^{-1403}$
JLM 8th	μ	2.77876×10^{-1}	2.77871×10^{-1}	2.77871×10^{-1}	2.77871×10^{-1}
	$\lvert\zeta(\mu)\rvert$	4.65450×10^{-5}	2.04096×10^{-31}	1.45092×10^{-189}	$1.87277 \times 10^{-1138}$

Table 4 Numerical results for Example 2, error fixed at $\delta = 10^{-3000}$ (Developed by the authors)

Methods	IG	N	FE	CPU Time
Proposed 8th	0.35	5	20	1.156
SM 8th	0.35	5	20	1.453
AKKB 8th	0.35	5	20	1.266
KBK 8th	0.35	5	20	2.313
JLM 8th	0.35	5	20	1.406

Example 3 (azeotropic point of a binary solution) [14], [29], [31]:

$$\zeta_3(\mu) = \frac{AB\left[B(1-\mu)^2 - A\mu^2\right]}{[\mu(A-B)+B]^2} \quad (31)$$

where A and B are coefficients in the Van Laar equation, which describes phase equilibria of liquid solutions. Consider for this problem that $A = 0.38969$ and $B = 0.55954$. The root of this equation is $\mu = 0.7573962463$. As an initial solution, we selected $\mu_0 = 0$.

Table 5 Numerical results for Example 3 for the first four iterations and their absolute function values at $\mu_0 = 0$ (Developed by the authors)

Methods	Iteration	1st Iteration	2nd Iteration	3rd Iteration	4th Iteration
Proposed 8th	μ	5.45213×10^{-1}	5.45098×10^{-1}	5.45098×10^{-1}	5.45098×10^{-1}
	$\lvert\zeta(\mu)\rvert$	1.08136×10^{-4}	8.93287×10^{-34}	1.93788×10^{-266}	$9.50623 \times 10^{-2128}$
SM 8th	μ	5.43841×10^{-1}	5.45098×10^{-1}	5.45098×10^{-1}	5.45098×10^{-1}
	$\lvert\zeta(\mu)\rvert$	2.10212×10^{-4}	9.23458×10^{-23}	1.32240×10^{-169}	$2.33842 \times 10^{-1344}$
AKKB 8th	μ	5.42440×10^{-1}	5.45098×10^{-1}	5.45098×10^{1}	5.45098×10^{-1}
	$\lvert\zeta(\mu)\rvert$	4.45921×10^{-4}	7.07655×10^{-22}	2.44038×10^{164}	$4.88144 \times 10^{-1304}$
KBK 8th	μ	6.59987×10^{-1}	5.45105×10^{-1}	5.45098×10^{-1}	5.45098×10^{-1}
	$\lvert\zeta(\mu)\rvert$	1.54022×10^{-2}	1.17287×10^{-6}	7.50379×10^{-41}	2.10601×10^{-314}
JLM 8th	μ	4.76022×10^{-1}	5.45096×10^{-1}	5.45098×10^{-1}	5.45098×10^{-1}
	$\lvert\zeta(\mu)\rvert$	1.32815×10^{-2}	2.16254×10^{-7}	1.03349×10^{-35}	1.23129×10^{-205}

Table 6 Numerical results for Example 3, error fixed at $\delta = 10^{-3000}$ (Developed by the authors)

Methods	IG	N	FE	CPU Time
Proposed 8th	0	5	20	0.781
SM 8th	0	5	20	1.422
AKKB 8th	0	5	20	1.359
KBK 8th	0	6	24	1.282
JLM 8th	0	6	24	1.531

Example 4 (Continuous Stirred Tank Reactor (CSTR)) [32]:

$$f_4(\mu) = \mu^4 + 11.50\mu^3 + 47.49\mu^2 + 83.06325\mu + 51.23266875 \quad (32)$$

Table 7 Numerical results for Example 4 for the first four iterations and their absolute function values at $\mu_0 = -1.5$ (Developed by the authors)

Methods	Iteration	1st Iteration	2nd Iteration	3rd Iteration	4th Iteration
Proposed 8th	μ	-1.45000×10^{0}	-1.45000×10^{0}	-1.45000×10^{0}	-1.45000×10^{0}
	$\lvert\zeta(\mu)\rvert$	1.14452×10^{-6}	2.43969×10^{-51}	1.03997×10^{-408}	$1.13376 \times 10^{-3267}$
SM 8th	μ	-1.44940×10^{0}	-1.45000×10^{0}	-1.45000×10^{0}	-1.45000×10^{0}
	$\lvert\zeta(\mu)\rvert$	1.42665×10^{5}	1.87984×10^{4}	2.45249×10^{3}	3.04714×10^{2}
AKKB 8th	μ	-1.37745×10^{0}	-1.09738×10^{0}	-1.33464×10^{0}	-1.42788×10^{0}
	$\lvert\zeta(\mu)\rvert$	4.67667×10^{-1}	3.52296×10^{0}	7.98753×10^{-1}	1.30706×10^{-1}
KBK 8th	μ	-1.45000×10^{0}	-1.45000×10^{0}	-1.45000×10^{0}	-1.45000×10^{0}
	$\lvert\zeta(\mu)\rvert$	4.48721×10^{-6}	1.86571×10^{-45}	1.66662×10^{-360}	$6.75742 \times 10^{-2881}$
JLM 8th	μ	-1.45000×10^{0}	-1.45000×10^{0}	-1.45000×10^{0}	-1.45000×10^{0}
	$\lvert\zeta(\mu)\rvert$	2.02305×10^{-6}	7.80637×10^{-38}	2.57694×10^{-226}	$3.33451 \times 10^{-1357}$

Table 8 Numerical results for Example 4, error fixed at $\delta = 10^{-3000}$ (Developed by the authors)

Methods	IG	N	FE	CPU Time
Proposed 8th	−1.5	4	16	0.907
SM 8th	−1.5	5	20	2.203
AKKB 8th	−1.5	9	36	2.813
KBK 8th	−1.5	5	20	2.062
JLM 8th	−1.5	5	20	2.547

5. Dynamics Study of the Methods

For investigating the stability of the proposed method at various initial guess we use the dynamical system, i.e., basin of attraction. If an algorithm fails to converge or converges to a different solution, it is considered inferior to the others. The main difficulty with this form of comparison is that the starting point is just one among an infinite number of possibilities. To combat this, the concept of a basin of attraction was developed. If a function contains n different zeroes (roots), the plane is split into n basins in an ideal case, and every basin has a different color. The basin of attraction method was initially discussed in [33]. Newton's approach was contrasted to Halley's, Popovski's, and Laguerre's third-order methods. This is preferable to comparing method by executing various non-linear functions with a certain initial value. Many articles have been published in the recent decade that use the concept of basin of attraction to compare the efficacy of various techniques.

6. Basin of Attraction for Proposed Algorithms

All basins are plotted with MATLAB R2018b within the range $\Re = [-1 \times 1] \times [-1 \times 1]$ with a density of $300 \times 300 = 90{,}000$ points. To terminate iterations, an error threshold of 1×10^{-10} or a maximum count of 100 iterations is chosen. Each point in $\Re$ is then picked as the starting condition for the algorithms. If the sequence generated by the iterative algorithm converges to a root x_k^* to the function $P_i(x)$ with the specified tolerance and iterations count $N \leq 100$, we decide to give the starting point a distinct color (not black) depending on the root it converged to. If the iterative algorithm starting with $x \in \Re$ transcends 100 iteration count before converging to any root x_k or converges to some other value, say p, with specified tolerance $|p - x^*| < 1 \times 10^{-10}$, we conclude that the starting point has diverged and a black is assigned to it.

The number of iterations is depicted for each point in another basin with a reference of a color bar alongside.

S. No.	Functions $(P(x))$	Roots $(x_k : k = 1,2,3,\ldots)$
1.	$P_1(x) = x^2 - \frac{1}{4}$	$x_k = \frac{1}{2}, -\frac{1}{2}$
2.	$P_2(x) = x^3 - \frac{1}{2}x^2 + \frac{1}{4}x - \frac{1}{8}$	$x_k = \frac{1}{2}, \frac{1}{2}i, -\frac{1}{2}i$
3.	$P_3(x) = x^3 + \frac{1}{16}x - \frac{5}{32}$	$x_k = \frac{1}{2}, -\frac{1}{4} \pm \frac{1}{2}i$
4.	$P_4(x) = x^4 + \frac{1}{64}$	$x_k = \frac{1 \pm 1i}{4}, \frac{-1 \pm 1i}{4}$
5.	$P_5(x) = x^5 - \frac{1}{2}ix^4 + \frac{1}{64}x - \frac{1}{128}i$	$x_k = \frac{1 \pm 1i}{4}, \frac{-1 \pm 1i}{4}, \frac{1}{2}i$
6.	$P_6(x) = x^2 - 1$	$x_k = 1, -1$

6.1. Basin of Attraction of the Proposed Eighth-Order Methods

The left figure shows roots while right figure shows the number of iterations at each initial point of $P_n(x)$ obtained by the proposed eighth-order method.

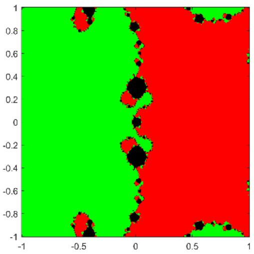
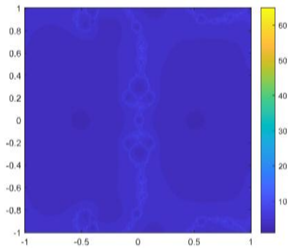

Fig. 1 Basin of attraction of $P_1(x)$ (Developed by authors)

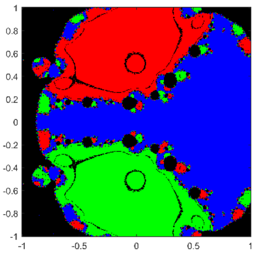
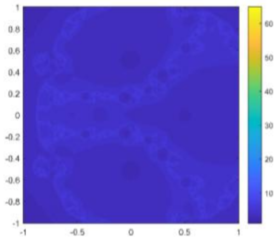

Fig. 2 Basin of attraction of $P_2(x)$ (Developed by authors)

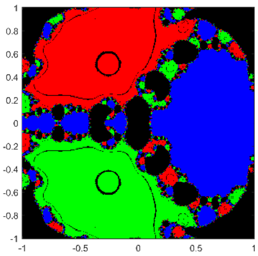
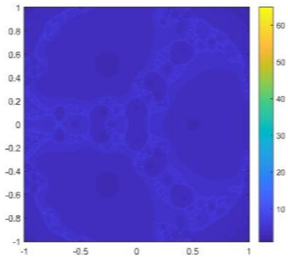

Fig. 3 Basin of attraction of $P_3(x)$ (Developed by authors)

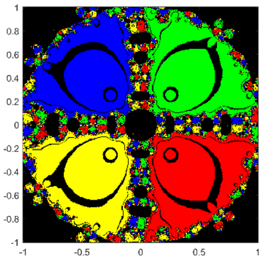
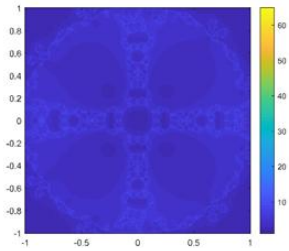

Fig. 4 Basin of attraction of $P_4(x)$ (Developed by authors)

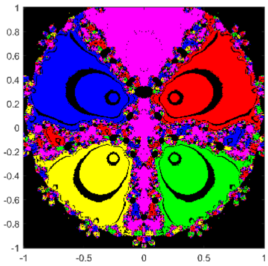
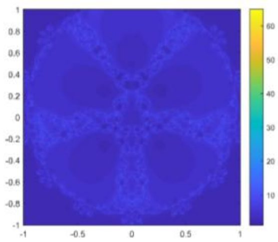

Fig. 5 Basin of attraction of $P_5(x)$ (Developed by authors)

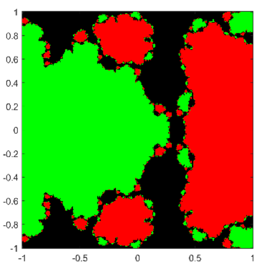
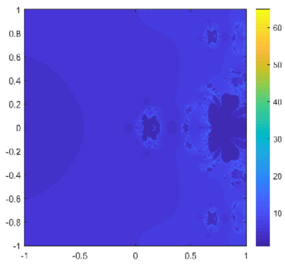

Fig. 6 Basin of attraction of $P_6(x)$ (Developed by authors)

Table 9 Comparison table (Developed by the authors)

Method	**Kong-ied [28] Method**	**Proposed Method**
Rate of convergence	8^{th}	8^{th}
Total function evaluations per iteration	5	4
Efficiency Index	1.515716567	1.681792831
Optimality	Non-optimal	Optimal

7. Conclusion

In this article, the main attention was focused upon to derive an optimal derivative free method of eight order with a three-step formula for finding the roots of non-linear equations in chemical engineering. Various application problems have been tested by the proposed method and compared with other available counterpart methods in the literature of the same order. For the analysis of the stability and consistency of the proposed method, the basin of attraction for various problems has been found to be suitable using the proposed method. It was observed from the comparison tables and basin of attraction in previous pages that the proposed eighth -order method is accurate, consistent, and their stability is robust compared to their counterpart methods available in the literature in all application problems. Therefore, the proposed method is one of the better alternate methods for the solution of nonlinear algebraic and transcendental equations. The implementation of the proposed method is all nonlinear algebraic and transcendental equations arise in various fields. In the future, we will propose a 16^{th}-order optimal derivative free method. Matlab, Mathematica 2021, and Maple 2021 software were used to obtain the results of various application problems and basin of attraction.

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Authors' Contributions

The authors approved the final manuscript. S. Jamali dealt with conceptualization and writing original draft preparation. Z. A. Kalhoro contributed to proper investigation and methodology. A. W. Shaikh dealt with the formal analysis and design. M. S. Chandio contributed to proper supervision and coordination.

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