



A Modified Twentieth-Order Iterative Method for Solving Nonlinear Physicochemical Models: Convergence, Physical Models and Basin of Attraction Analysis

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Abstract: This paper introduces a modified twentieth-order method for solving nonlinear equations that commonly arise in physicochemical models. The proposed method is designed to efficiently handle the complex problems that normally occur in the van der Waals equation for real gases, Planck's radiation law, and chemical equilibrium conditions. The traditional method has a lower order of convergence and uses higher-order derivatives. However, proposed method has twentieth-order convergence with only one first derivative used in each iteration. A detailed convergence order has been carried out to demonstrate the theoretical order of accuracy. Various numerical experiments have also been carried out to validate the performance of the proposed method. The results show the significantly improve the accuracy and taking a smaller number of iterations, number of function evaluations, and CPU time when applied to nonlinear equations arises in van der Waals equation for real gases, Planck's radiation law, and chemical equilibrium conditions and basin of attraction further validate the stability of proposed method.

Keywords: Nonlinear Physicochemical Models, Iterative Method, Convergence Analysis, Weight Function, Hermite Interpolation, Basin of Attraction.

1. INTRODUCTION

One of the key challenges in numerical analysis is solving nonlinear equations that arise in engineering problems, specifically in arises in van der Waals equation for real gases, Planck's radiation law, and chemical equilibrium conditions. Iterative methods, like newton's method, are commonly employed for this purpose. In this context, this article focuses on iterative techniques aimed at finding a simple root a , such that $\psi(a) = 0$ and $\psi'(a) \neq 0$, for a nonlinear equation $\psi(x) = 0$ [1]. High precision is most significant for numerical

computation, highlighting the importance of higher-order numerical methods [2]. Many scholars have proposed higher-order methods for solving nonlinear algebraic and transcendental equations [3-5]. Similarly, a number of researchers have also introduced a higher-order convergence optimal method [6-8]. Bracketing/closed method [9-13] have also have their importance because they have always been convergent, but their convergence is very slow. So now the researchers are more intend to introduce higher order method using weight function techniques [14-16].

2. DERIVATION

We use the Newton technique [1] as the first step in the suggested approach.

$$v_n = \kappa_n - \frac{\psi(\kappa_n)}{\psi'(\kappa_n)} \quad (1)$$

In the second step of the proposed method, we utilize a variant of the double Newton method [17] and modify it by substituting $\psi(\kappa_n)$ with $\psi'(\kappa_n)$ in this step.

$$\xi_n = v_n - \left[1 + \left(\frac{\psi(v_n)}{\psi'(\kappa_n)} \right)^2 \right] \left(\frac{\psi(v_n)}{\psi'(v_n)} \right) \quad (2)$$

From Equations (1) and (2) we get:

$$\left. \begin{array}{l} \text{Step 1. } v_n = \kappa_n - \frac{\psi(\kappa_n)}{\psi'(\kappa_n)} \\ \text{Step 2. } \xi_n = v_n - \left[1 + \left(\frac{\psi(v_n)}{\psi'(\kappa_n)} \right)^2 \right] \left(\frac{\psi(v_n)}{\psi'(v_n)} \right) \end{array} \right\} \quad (3)$$

To enhance the accuracy and convergence, introduce the weight function L see in Thukral [18] in the step 2 of Equation (3).

$$\text{Where } L = K - 2a + 2ab(a-1)^2 + 2a^3b^{-1} \\ \text{And } K = (1 - a^2 - 10a^4)^{-1}, \quad a = \frac{\psi(v_n)}{\psi(\kappa_n)}, \quad b = \frac{\psi'(\kappa_n)}{\psi'(v_n)}$$

We get

$$\left. \begin{array}{l} \text{Step 1. } v_n = \kappa_n - \frac{\psi(\kappa_n)}{\psi'(\kappa_n)} \\ \text{Step 2. } \xi_n = v_n - L \left[1 + \left(\frac{\psi(v_n)}{\psi'(\kappa_n)} \right)^2 \right] \left(\frac{\psi(v_n)}{\psi'(v_n)} \right) \end{array} \right\} \quad (4)$$

And add one more step of newton by using $\psi(\xi_n)$ and $\psi'(\xi_n)$, $\psi'(\xi_n) \approx h'_3(\xi_n)$

$$\left. \begin{array}{l} \text{Step 1. } v_n = \kappa_n - \frac{\psi(\kappa_n)}{\psi'(\kappa_n)} \\ \text{Step 2. } \xi_n = v_n - L \left[1 + \left(\frac{\psi(v_n)}{\psi'(\kappa_n)} \right)^2 \right] \left(\frac{\psi(v_n)}{\psi'(v_n)} \right) \\ \text{Step 3. } o_n = \xi_n - \frac{\psi(\xi_n)}{\psi'(\xi_n)} \end{array} \right\} \quad (5)$$

In three-step formula mentioned in Equation (5) we estimate $\psi'(\xi_n)$ using existing data, thereby reducing the number of function evaluations needed per iteration. At the nodes κ , v , and ξ , we have four values $\psi(\kappa)$, $\psi'(\kappa)$, $\psi(v)$ and $\psi(\xi)$. In the third step of the iterative scheme in Equation (5), we use the approximation $\psi'(\xi) \approx H'_3(\xi)$ to approximate ψ using Hermite's interpolating polynomial of degree 3. This algorithm takes the following form.

$$H_3(\eta) = a_0 + a_1(\eta - \kappa) + a_2(\eta - \kappa)^2 + a_3(\eta - \kappa)^3 \quad (6)$$

And its derivative is:

$$H'_3(\eta) = a_1 + 2a_2(\eta - \kappa) + 3a_3(\eta - \kappa)^2 \quad (7)$$

The unknown coefficients will be determined using available data from the conditions:

$$H_3(\kappa) = \psi(\kappa), \quad H_3(v) = \psi(v), \quad H_3(\xi) = \psi(\xi) \\ \& H'_3(\kappa) = \psi'(\kappa).$$

Putting $\eta = \kappa$ into Equations (6) and (7) we get $a_0 = \psi(\kappa)$ and $a_1 = \psi'(\kappa)$. The coefficients a_2 and a_3 are obtained from the system of two linear equations formed by using the remaining two conditions $\eta = v$ & $\eta = \xi$ in Equation (6) and we obtain:

$$a_2 = \frac{(\xi - \kappa)\psi[v, \kappa]}{(\xi - v)(v - \kappa)} - \frac{(v - \kappa)\psi[\xi, \kappa]}{(\xi - v)(v - \kappa)} - \psi'(\kappa) \left(\frac{1}{\xi - \kappa} - \frac{1}{v - \kappa} \right)$$

$$\& a_3 = \frac{\psi[\xi, \kappa]}{(\xi - v)(\xi - \kappa)} - \frac{\psi[v, \kappa]}{(\xi - v)(v - \kappa)} + \frac{\psi'(\kappa)}{(\xi - \kappa)(v - \kappa)}$$

By putting the values of a_1, a_2, a_3 & $\eta = \xi$ in Equation (7) we get:

$$H'_3(\xi) = 2(\psi[\kappa, \xi] - \psi[\kappa, v]) + \psi[v, \xi] + \frac{v - \xi}{v - \kappa} (\psi[v, v] - \psi'(\kappa)) \quad (8)$$

We replace $\psi'(\xi_n)$ in third step of Equation (5) by Equation (8) H_3 Hermite we get:

$$\left. \begin{array}{l} \text{Step 1. } v_n = \kappa_n - \frac{\psi(\kappa_n)}{\psi'(\kappa_n)} \\ \text{Step 2. } \xi_n = v_n - L \left[1 + \left(\frac{\psi(v_n)}{\psi'(\kappa_n)} \right)^2 \right] \left(\frac{\psi(v_n)}{\psi'(v_n)} \right) \\ \text{Step 3. } o_n = \xi_n - \frac{\psi(\xi_n)}{h'_3(\xi_n)} \end{array} \right\} \quad (9)$$

Now add one more step of newton by using $\psi(o_n)$ and $\psi'(o_n)$

And finally, we got

$$\left. \begin{array}{l} \text{Step 1. } v_n = \kappa_n - \frac{\psi(\kappa_n)}{\psi'(\kappa_n)} \\ \text{Step 2. } \xi_n = v_n - L \left[1 + \left(\frac{\psi(v_n)}{\psi'(\kappa_n)} \right)^2 \right] \left(\frac{\psi(v_n)}{\psi'(v_n)} \right) \\ \text{Step 3. } o_n = \xi_n - \frac{\psi(\xi_n)}{h'_3(\xi_n)} \\ \text{Step 4. } \kappa_{n+1} = o_n - \frac{\psi(o_n)}{\psi'(o_n)} \end{array} \right\} \quad (10)$$

Equation (10) is the twentieth-order method with four function evaluations and three first derivatives.

3. CONVERGENCE ANALYSIS

Theorem: D represents an open interval containing κ_0 as a first estimate of $\sigma \in D$. Let $\sigma \in D$ be a simple root of a function $\psi : D \subset R \rightarrow R$ that is suitably differentiable. Under these conditions, Equation (10) yields Twentieth-order of convergence and requires only four function evaluations along with three first derivative calculations in each complete iteration, with no need for second or higher-order derivatives.

Proof.

The Taylor series expansion for the function $\psi(\kappa_n)$ can be expressed as:

$$\begin{aligned} \psi(\kappa_n) &= \sum_{m=0}^{\infty} \frac{\psi^m(\sigma)}{m!} (\kappa_n - \sigma)^m = \psi(\sigma) + \\ &\quad \psi'(\sigma)(\kappa_n - \sigma) + \frac{\psi''(\sigma)}{2!} (\kappa_n - \sigma)^2 + \\ &\quad \frac{\psi'''(\sigma)}{3!} (\kappa_n - \sigma)^3 + \dots \end{aligned} \quad (11)$$

For simplicity, we assume that $R_k = \left(\frac{1}{k!} \right) \frac{\psi^k(\sigma)}{\psi'(\sigma)}$, $k \geq 2$.

and assume that $\varepsilon_n = \kappa_n - \sigma$. Thus, we have:

For step one:

$$\psi(\kappa_n) = \psi'(\sigma) \left(\varepsilon_n + R_2 \varepsilon_n^2 + R_3 \varepsilon_n^3 + \dots + R_4 \varepsilon_n^4 + \dots + R_{21} \varepsilon_n^{21} \right) \quad (12)$$

$$\psi'(\kappa_n) = \psi'(\sigma) \left(1 + 2R_2 \varepsilon_n + 3R_3 \varepsilon_n^2 + \dots + 4R_4 \varepsilon_n^3 + \dots + 21R_{21} \varepsilon_n^{20} \right) \quad (13)$$

From Equations (12) and (13):

$$\text{Step 1. } \nu_n = \kappa_n - \frac{\psi(\kappa_n)}{\psi'(\kappa_n)} = R_2 \varepsilon_n^2 + (2R_3 - 2R_2^2) \varepsilon_n^3 + (4R_2^3 - 7R_3 R_2 + 3R_4) \varepsilon_n^4 + \dots + O(\varepsilon_n^{21}) \quad (14)$$

$$\text{Step 2. } \xi_n = \nu_n - L * \left(1 + \left(\frac{\psi(\nu_n)}{\psi'(\nu_n)} \right)^2 \right) \left(\frac{\psi(\nu_n)}{\psi'(\nu_n)} \right) = R_2^2 (3R_2^3 - (7R_3 + 1)R_2 + R_4) \varepsilon_n^6 - 2 \left(R_2 \left(\frac{R_2^5 - (36R_3 + 5)R_2^3 + 9R_4 R_2^2 +}{(R_3(20R_3 + 3) - R_5)R_2 - 2R_3 R_4} \right) \right) \varepsilon_n^7 + \dots + O(\varepsilon_n^{21}) \quad (15)$$

$$\text{Step 3. } o_n = \xi_n - \frac{\psi(\xi_n)}{h_3'(\xi)} =$$

$$\begin{aligned} & R_2^3 R_4 (3R_2^3 - (7R_3 + 1)R_2 + R_4) \varepsilon_n^{11} + \\ & R_2^2 \left(\frac{2R_2 (3R_2^3 - (7R_3 + 1)R_2 + 2R_4) R_5 -}{2R_4 \left(4R_2^5 - 2(23R_3 + 3)R_2^3 + 10R_4 R_2^2 + \right)} \right) \varepsilon_n^{12} + \\ & \dots + O(\varepsilon_n^{21}) \end{aligned} \quad (16)$$

$$\text{Step 4. } \kappa_{n+1} = o_n - \frac{\psi(o_n)}{\psi'(o_n)} = R_2^7 R_4^2 (3c_2^3 - (7R_3 + 1)R_2 + R_4)^2 \varepsilon_n^{20} + O(\varepsilon_n^{21}) \quad (17)$$

Lastly, the efficiency index of the proposed approach mentioned in Equation (10) is 1.534127405, the rate of convergence is twenty, and each iteration requires three first derivative evaluations and four function evaluations.

4. NUMERICAL EXPERIMENT AND DISCUSSION

Problem 1. A chemical equilibrium problem(see [19-21]).

$$\kappa^4 - 7.79075\kappa^3 + 14.7445\kappa^2 + 2.511\kappa - 1.674 = 0$$

Table 1. Numerical results for problem 1 for first four iterations and their absolute function values at $\kappa_0 = 0.6$.

Method	Root & absolute function value	1 st iteration	2 nd iteration	3 rd iteration	4 th iteration
PM	κ $ \psi(\kappa) $	0.2777 ... 3.9356E - 13	0.2777 ... 2.9239E - 267	0.2777 ... 7.6755E - 5350	0.2777 ... 1.8529E - 107001
A1 20 th	κ $ \psi(\kappa) $	0.2777 ... 5.0042E - 11	0.2777 ... 1.2188E - 221	0.2777 ... 6.5800E - 4434	0.2777 ... 2.9086E - 88679
A2 20 th	κ $ \psi(\kappa) $	0.2777 ... 2.2287E - 10	0.2777 ... 5.0928E - 208	0.2777 ... 7.6768E - 4161	0.2777 ... 2.8154E - 83217
A3 20 th	κ $ \psi(\kappa) $	0.2777 ... 1.6868E - 10	0.2777 ... 1.4682E - 210	0.2777 ... 9.1397E - 4212	0.2777 ... 6.9775E - 83236

Table 2. Numerical results for the problem 1, error fixed at $\delta = 1 \times 10^{-5}$.

Method	IG	N	FE	CPU Time
PM	0.6	4	28	2.78×10^0
A1 20 th	0.6	5	35	8.39×10^0
A2 20 th	0.6	5	35	9.56×10^0
A3 20 th	0.6	5	35	1.02×10^1

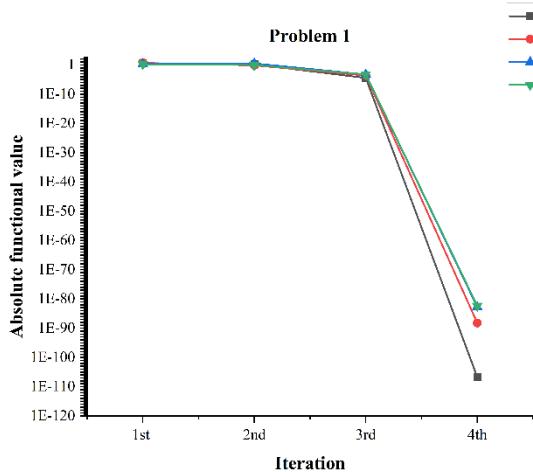


Fig. 1. Graphical Representation of $|\psi(\kappa)|$ of Table 1. by assuming the scale $1 \times 10^{-3} = 1 \times 10^{-1}$.

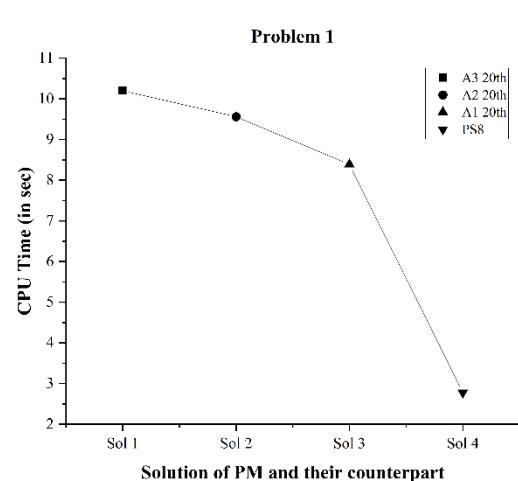


Fig. 2. CPU time (in sec) versus solution of problem 1 by the proposed scheme and its counterparts.

The performance of the PM method in solving problem 1 is evaluated against A1 20th, A2 20th, and A3 20th up to the fourth iteration. Results presented in Table 1 indicate that PM achieves higher accuracy and faster convergence, as depicted in Figure 1, which illustrates PM's quicker convergence relative to the other methods. Table 2 provides detailed metrics, showing that PM requires only 4 iterations and 28 function evaluations, whereas the other methods necessitate 5 iterations and 35 evaluations. Additionally, PM consumes less CPU time to achieve a tolerance of 1×10^{-5} , with Figure 2 reinforcing its superior CPU time performance compared to alternative methods.

Problem 2. Volume from van der Waals equation (see [8])

$$\psi(\kappa) = 40\kappa^3 - 95.26535116\kappa^2 + 35.28\kappa - 5.6998368$$

Table 3. Numerical results for problem 2 for first four iterations and their absolute function values at $\kappa_0 = 2.5$.

Method	Root & absolute functional value	1 st iteration	2 nd iteration	3 rd iteration	4 th iteration
PM	κ $ \psi(\kappa) $	1.9707 ... 2.7230E - 7	1.9707 ... 7.3008E - 207	1.9707 ... 1.3896E - 4996	1.9707 ... 7.1118E - 119950
A1 20 th	κ $ \psi(\kappa) $	1.9707 ... 8.3409E - 5	1.9707 ... 1.4913E - 118	1.9707 ... 1.6624E - 2393	1.9707 ... 1.4603E - 47892
A2 20 th	κ $ \psi(\kappa) $	1.9707 ... 4.2265E - 5	1.9707 ... 8.9428E - 125	1.9707 ... 2.8928E - 2518	1.9707 ... 4.5534E - 50388
A3 20 th	κ $ \psi(\kappa) $	1.9707 ... 5.1315E - 5	1.9707 ... 5.3469E - 123	1.9707 ... 1.2172E - 2482	1.9707 ... 1.7007E - 49675

Table 4. Numerical results for problem 2, error fixed at $\delta = 1 \times 10^{-5}$.

Method	IG	N	FE	CPU Time
PM	2.5	4	28	7.08×10^0
A1 20 th	2.5	5	35	7.32×10^0
A2 20 th	2.5	5	35	7.94×10^0
A3 20 th	2.5	5	35	7.78×10^0

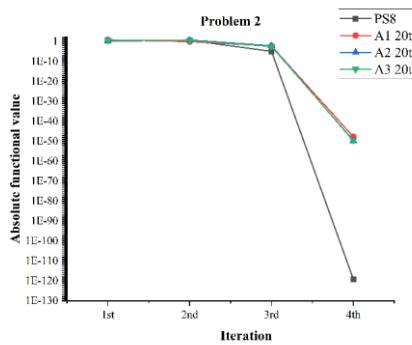
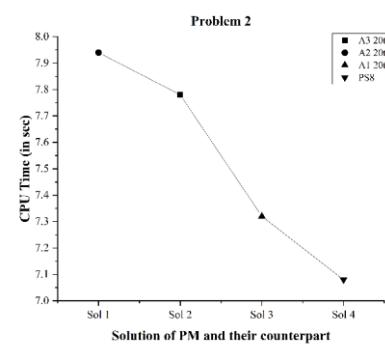

Fig. 3. Graphical Representation of $|\psi(\kappa)|$ of Table 3. by assuming the scale $1 \times 10^{-3} = 1 \times 10^{-1}$.

Fig. 4. CPU time versus the solution of problem 2 with the proposed scheme and its counterparts.

Table 3 shows that PM is more accurate and converges quickly than its counterpart approaches in problem 2. And Table 4 shows the iterations, function evaluations, and CPU time (in seconds), where A1, A2, and A3 need 5 iterations and 35 function evaluations, whereas PM requires 4 and 28. PM achieves a tolerance of $\delta = 1 \times 10^{-5}$ more effectively than comparable approaches because of its decreased CPU time (in seconds). However, Figures 3 and 4 are graphical representations of Tables 3 and 4, also demonstrating that the proposed method is more accurate.

Problem 3. Planck's radiation law (see [20, 22-25, 27]).

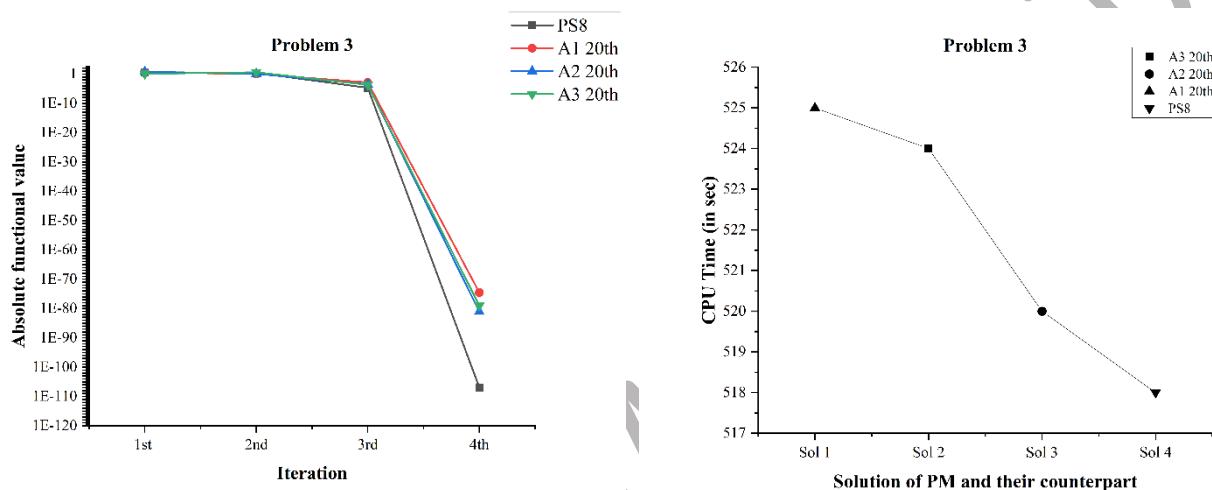
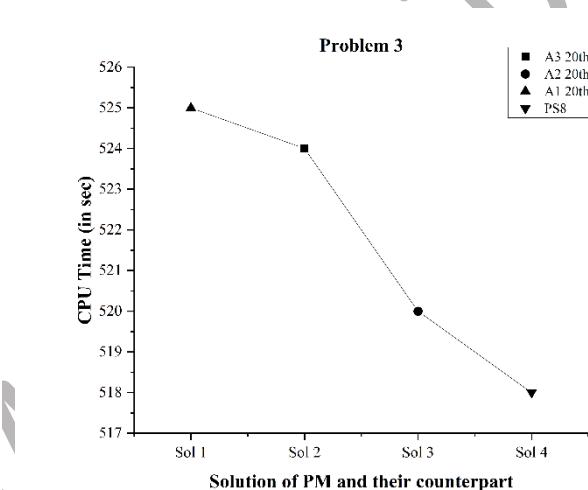
$$e^{-\kappa} - 1 + \frac{\kappa}{5} = 0.$$

Table 5. Numerical results for problem 3 for first four iterations and their absolute function values at $\kappa_0 = -0.5$.

Method	absolute functional value	Root &			
		1 st iteration	2 nd iteration	3 rd iteration	4 th iteration
PM	$ \psi(\kappa) $	-5.9344E - 14 4.7475E - 14	-1.6768E - 269 4.7475E - 269	-1.7657E - 5380 4.7475E - 5380	-4.9576E - 107600 4.7475E - 107600
A1 20 th	$ \psi(\kappa) $	-5.4708E - 10 4.3767E - 10	-2.0950E - 187 1.6760E - 187	-9.6359E - 3736 7.7087E - 3736	-1.7293E - 74702 1.3835E - 74702
A2 20 th	$ \psi(\kappa) $	-7.6741E - 11 6.1393E - 11	-2.5011E - 205 2.0009E - 205	-2.5011E - 4095 3.6606E - 4095	-8.0702E - 81890 6.4562E - 81890
A3 20 th	$ \psi(\kappa) $	-1.5682E - 10 1.2545E - 10	-8.2960E - 199 6.6368E - 199	-2.4446E - 3964 1.9556E - 3964	-5.9562E - 79275 1.9556E - 79275

Table 6. Numerical results for problem 3, error fixed at $\delta = 1 \times 10^{-5}$.

Method	IG	N	FE	CPU Time
PM	-0.5	4	28	5.18×10^2
A1 20 th	-0.5	5	35	5.25×10^2
A2 20 th	-0.5	5	35	5.20×10^2
A3 20 th	-0.5	5	35	5.24×10^2


Fig. 5. Graphical Representation of $|\psi(\kappa)|$ of Table 5. by assuming the scale $1 \times 10^{-3} = 1 \times 10^{-1}$.

Fig. 6. CPU time (in sec) versus solution of problem 3 with the proposed scheme and its counterparts.

Compared to its counterpart approaches in problem 3, PM is more accurate and converges faster, as Table 5 demonstrates. Additionally, Table 6 displays the CPU time (in seconds), number of iterations, function evaluations. A1, A2, and A3 require five iterations and thirty-five function evaluations, while PM needs four and twenty-eight. PM's reduced CPU time (in seconds) allows it to achieve a tolerance of $\delta = 1 \times 10^{-5}$ more efficiently than similar methods. Figures 3 and 4, on the other hand, are graphical depictions of Tables 5 and 6, further proving the validity of the suggested approach.

The visuals show that PM is more accurate, efficient, and consistent than alternative approaches.

5. BASIN OF ATTARCTION

The stability of the solutions (roots) for the nonlinear function $\psi(\kappa) = 0$. The concept of basins of attraction can be used to facilitate an iterative method [26]. MATLAB R2014a was used to generate a depiction of all basins within the range $R = [-5 \times 5] \times [-5 \times 5]$, with a total of 360,000 points at a 600×600 density. There were two criteria established: An error threshold of 1×10^{-10} or a maximum iteration count of 10. Each point in the R-range served as the starting condition for the iterative algorithms that are initiated.

Problem 4. Below problems were taken from the literature [26].

S. No	Functions ($P(x)$)	Roots ($x_k : k = 1, 2, 3, \dots$)
1.	$P_1(x) = x^5 + 1$	$x_k = -1, -\frac{305}{987} \pm \frac{855}{899}i, \frac{1292}{1597} \pm \frac{4456}{7581}i$
2.	$P_2(x) = x^3 + 1$	$x_k = 1, \frac{1 \pm \sqrt{3}i}{2}$
3.	$P_3(x) = x^2 + 2x - \frac{1}{2}$	$x_k = \frac{-2 \pm \sqrt{6}}{2}$

4. $P_4(x) = x^4 + \frac{1}{64}$

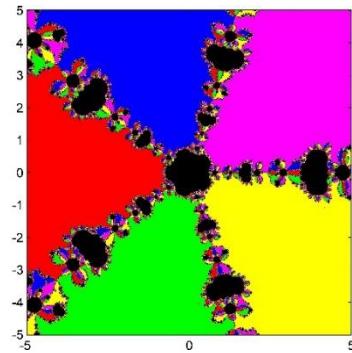
5. $P_5(x) = x^5 - \frac{1}{2}ix^4 + \frac{1}{64}x - \frac{1}{128}i$

6. $P_6(x) = x^2 - \frac{1}{4}$

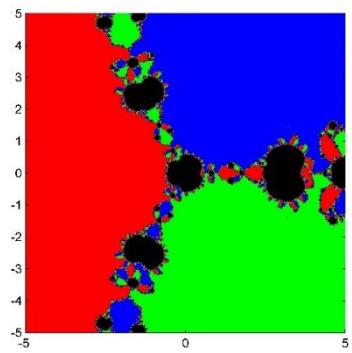
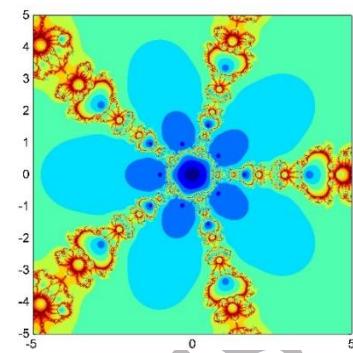
$$x_k = \frac{1 \pm 1i}{4}, \frac{-1 \pm 1i}{4}$$

$$x_k = \frac{1 \pm 1i}{4}, \frac{-1 \pm 1i}{4}, \frac{1}{2}i$$

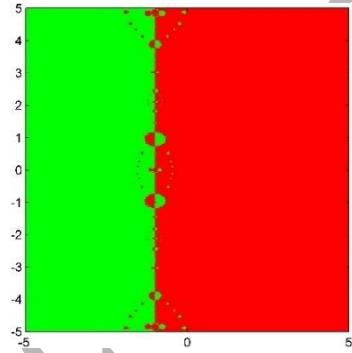
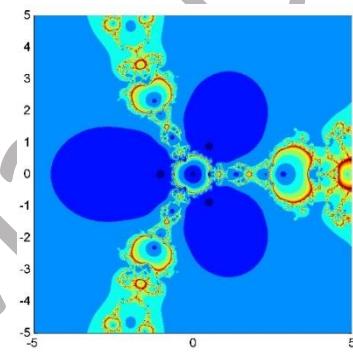
$$x_k = \frac{1}{2}, -\frac{1}{2}$$



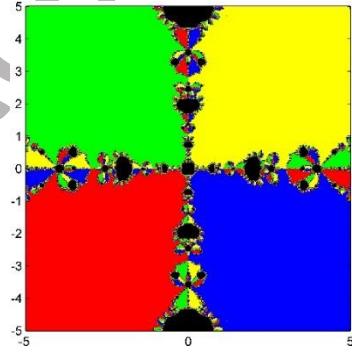
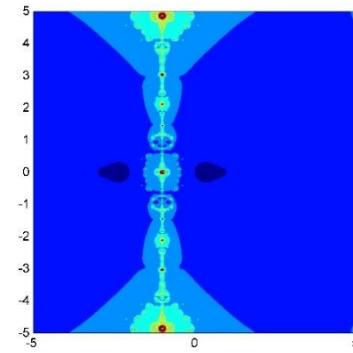
Basin of attraction of $P_1(x)$



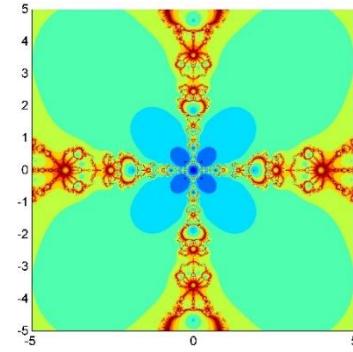
Basin of attraction of $P_2(x)$



Basin of attraction of $P_3(x)$



Basin of attraction of $P_4(x)$



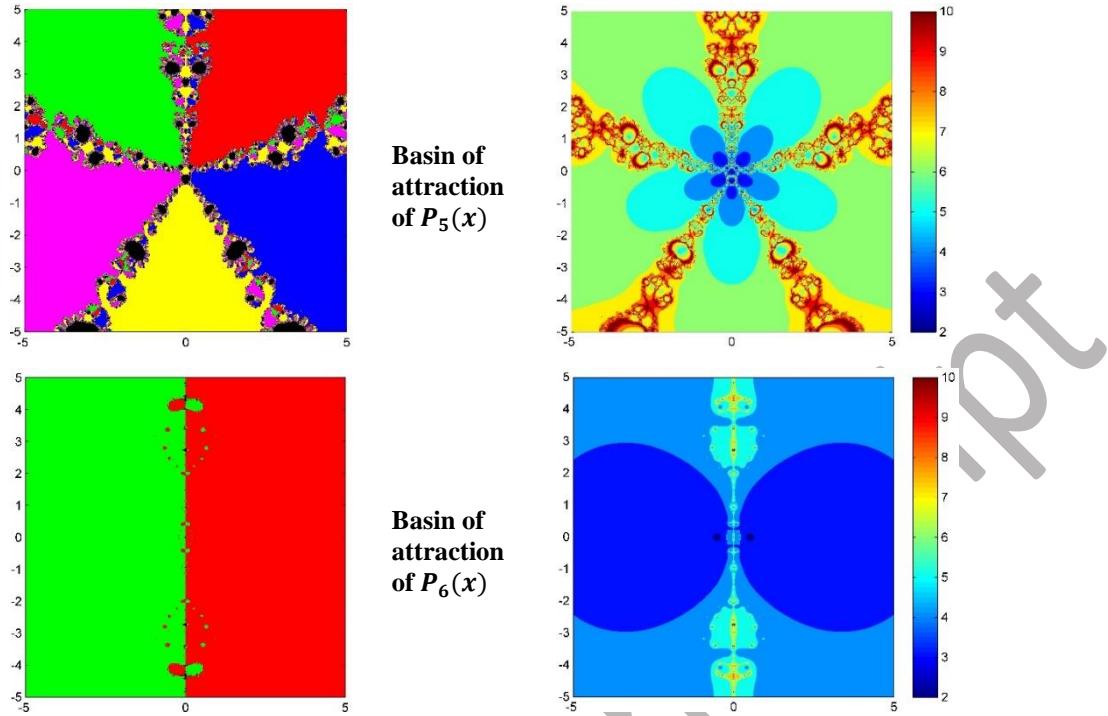


Fig. 7. The left Figures shows roots, while the right Figures. shows the number of iterations at each initial point of $P_n(x)$ of problems 4 obtained by the proposed Twentieth-order method.

The iterative algorithm assigned a unique color number k (other than black) to the initial point if the sequence converged to a root x_k^* of the polynomial $P_n(x)$ of degree k within 10 iterations and a predetermined tolerance. On the other hand, if the iterative process started at a point $x \in C$ and surpassed the maximum iteration limit of 10 without converging to any root x_k or converged to a different value p such that $|p - x^*| < 1 \times 10^{-10}$, the starting point was classified as diverging. In these instances, the starting point was marked with the color black. The number of iterations for each point in another basin is represented, accompanied by a color scale for reference.

The visual representations presented above show that PM has significantly higher stability than alternative methods.

6. CONCLUSIONS

The proposed fourth step, the twenty-order method based on the weight function, is introduced for the solution of nonlinear equations arising in Physicochemical Models. In conclusion, we have derived the convergence order (theoretical) of the proposed method, various application problems from the Physicochemical Models have been tested and compared with counterparts A1, A2, and A3. In all cases proposed method outperforms existing methods in terms of accuracy, number of iterations, number of function evaluations, and CPU time.

Furthermore, the Basin of attraction in the complex plane confirms the stability of the proposed method.

7. CONFLICTS OF INTEREST

The authors declare no conflict of interest.

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