



# 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.



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:

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

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:

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

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

From Equations (12) and (13):

$$\text{Step 1. } v_n = \kappa_n - \frac{\psi(\kappa_n)}{\psi'(\kappa_n)} = R_2 \varepsilon_n^2 + (2R_3 - 2R_2^2) \varepsilon_n^3 +$$

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

$$(4R_2^3 - 7R_3 R_2 + 3R_4) \varepsilon_n^4 + \dots + O(\varepsilon_n^{21}) \quad (14)$$

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

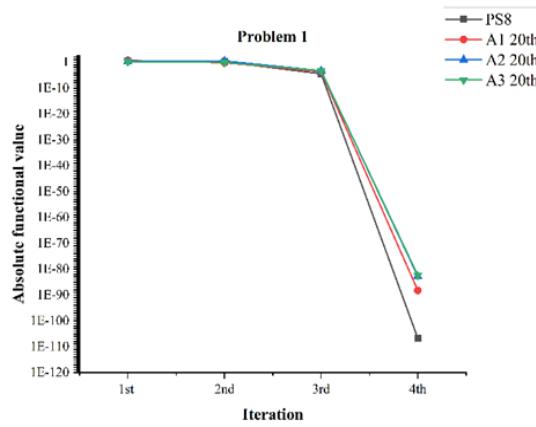
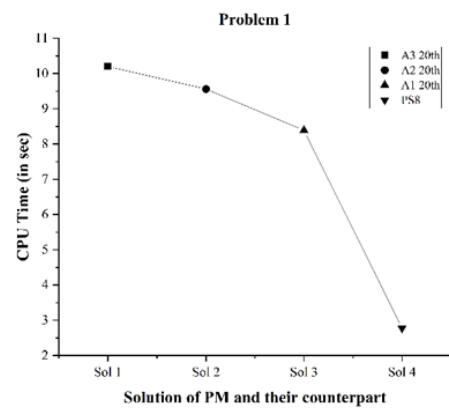
$$\begin{aligned}\text{Step 3. } o_n &= \xi_n - \frac{\psi(\xi_n)}{h_3'(\xi)} = \\ &\quad R_2^3 R_4 (3R_2^3 - (7R_3 + 1)R_2 + R_4) \varepsilon_n^{11} + \\ &\quad 2R_2 \left( \frac{2R_2 (3R_2^3 - (7R_3 + 1)R_2 + 2R_4) R_5 -}{2R_4 (4R_2^5 - 2(23R_3 + 3)R_2^3 + 10R_4 R_2^2 +)} \right) \varepsilon_n^{12} + \\ &\quad \dots + O(\varepsilon_n^{21}) \quad (16)\end{aligned}$$

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

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.

**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	$2.78 \times 10^0$
A1 20 <sup>th</sup>	0.6	5	35	$8.39 \times 10^0$
A2 20 <sup>th</sup>	0.6	5	35	$9.56 \times 10^0$
A3 20 <sup>th</sup>	0.6	5	35	$1.02 \times 10^1$

**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 20<sup>th</sup>, A2 20<sup>th</sup>, and A3 20<sup>th</sup> 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  $1 \times 10^{-5}$ , 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 <sup>st</sup> iteration	2 <sup>nd</sup> iteration	3 <sup>rd</sup> iteration	4 <sup>th</sup> iteration
PM	$\kappa$	1.9707 ...	1.9707 ...	1.9707 ...	1.9707 ...
	$ \psi(\kappa) $	2.7230E - 7	7.3008E - 207	1.3896E - 4996	7.1118E - 119950
A1 20 <sup>th</sup>	$\kappa$	1.9707 ...	1.9707 ...	1.9707 ...	1.9707 ...
	$ \psi(\kappa) $	8.3409E - 5	1.4913E - 118	1.6624E - 2393	1.4603E - 47892
A2 20 <sup>th</sup>	$\kappa$	1.9707 ...	1.9707 ...	1.9707 ...	1.9707 ...
	$ \psi(\kappa) $	4.2265E - 5	8.9428E - 125	2.8928E - 2518	4.5534E - 50388
A3 20 <sup>th</sup>	$\kappa$	1.9707 ...	1.9707 ...	1.9707 ...	1.9707 ...
	$ \psi(\kappa) $	5.1315E - 5	5.3469E - 123	1.2172E - 2482	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	$7.08 \times 10^0$
A1 20 <sup>th</sup>	2.5	5	35	$7.32 \times 10^0$
A2 20 <sup>th</sup>	2.5	5	35	$7.94 \times 10^0$
A3 20 <sup>th</sup>	2.5	5	35	$7.78 \times 10^0$

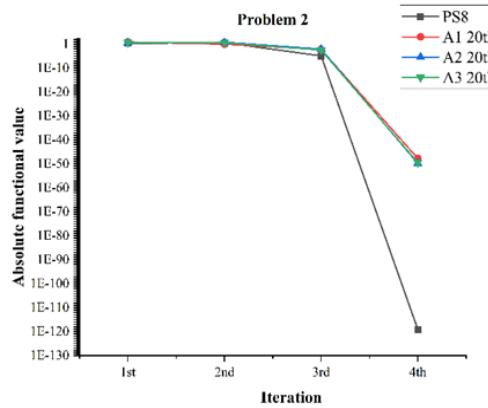
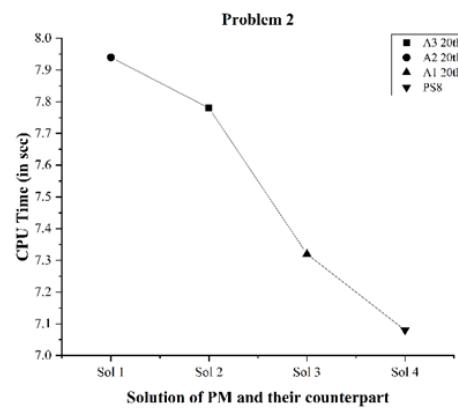
**Fig. 3.** Graphical Representation of  $|\psi(\kappa)|$  of Table 3. by assuming the scale  $1 \times 10^{-3} = 1 \times 10^{-1}$ .**Fig. 4.** CPU time versus the solution of problem 2 with the proposed scheme and its counterparts.

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])

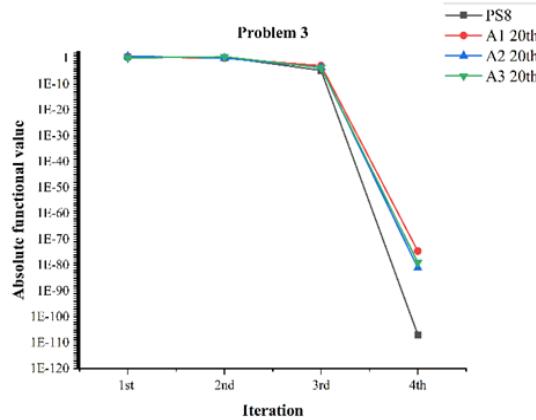
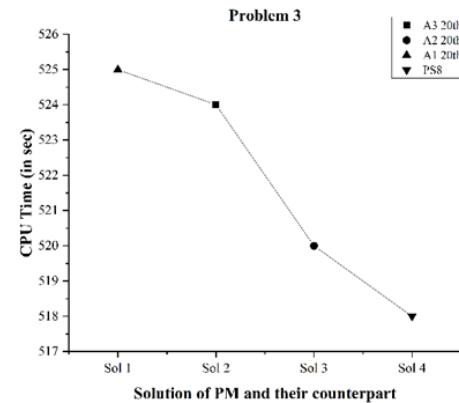
$$e^{-\kappa} - 1 + \frac{\kappa}{5} = 0.$$

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

Method	Root & absolute functional value	1 <sup>st</sup> iteration	2 <sup>nd</sup> iteration	3 <sup>rd</sup> iteration	4 <sup>th</sup> iteration
PM	$\kappa$	-5.9344E - 14	-1.6768E - 269	-1.7657E - 5380	-4.9576E - 107600
	$ \psi(\kappa) $	4.7475E - 14	4.7475E - 269	4.7475E - 5380	4.7475E - 107600
A1 20 <sup>th</sup>	$\kappa$	-5.4708E - 10	-2.0950E - 187	-9.6359E - 3736	-1.7293E - 74702
	$ \psi(\kappa) $	4.3767E - 10	1.6760E - 187	7.7087E - 3736	1.3835E - 74702
A2 20 <sup>th</sup>	$\kappa$	-7.6741E - 11	-2.5011E - 205	-2.5011E - 4095	-8.0702E - 81890
	$ \psi(\kappa) $	6.1393E - 11	2.0009E - 205	3.6606E - 4095	6.4562E - 81890
A3 20 <sup>th</sup>	$\kappa$	-1.5682E - 10	-8.2960E - 199	-2.4446E - 3964	-5.9562E - 79275
	$ \psi(\kappa) $	1.2545E - 10	6.6368E - 199	1.9556E - 3964	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	$5.18 \times 10^2$
A1 20 <sup>th</sup>	-0.5	5	35	$5.25 \times 10^2$
A2 20 <sup>th</sup>	-0.5	5	35	$5.20 \times 10^2$
A3 20 <sup>th</sup>	-0.5	5	35	$5.24 \times 10^2$

**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  $600 \times 600$  density. There were two criteria established: An error threshold of  $1 \times 10^{-10}$

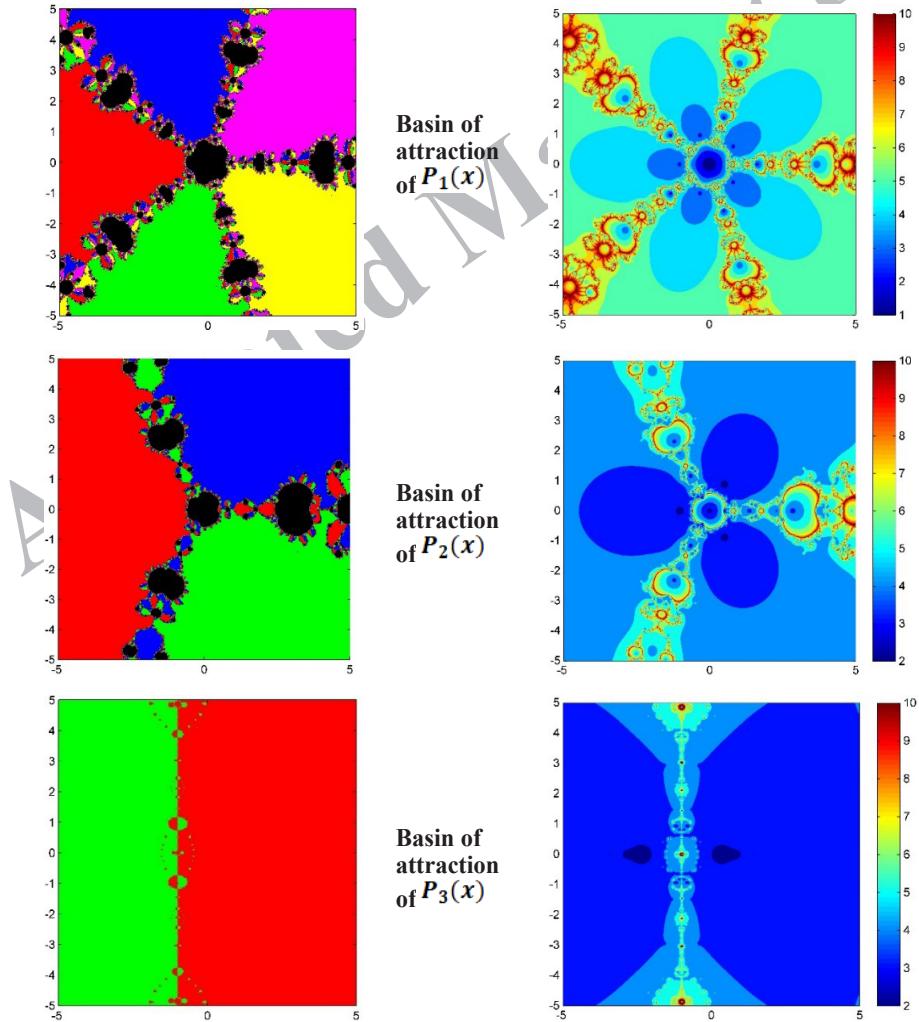
or a maximum iteration count of 10. Each point in the R-range served as the starting condition for the iterative algorithms that are initiated.

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.

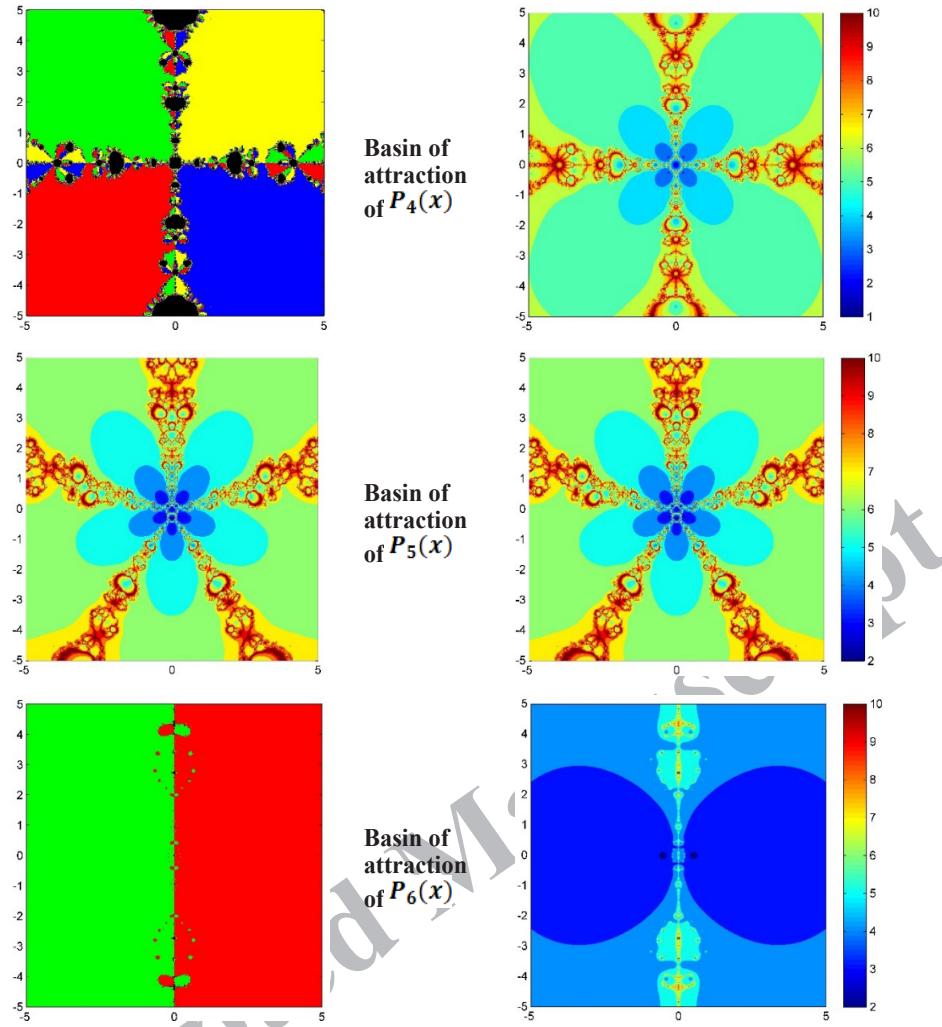
The visual representations presented in Figure 7 show that PM has significantly higher stability than alternative methods.

**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.	$P_4(x) = x^4 + \frac{1}{64}$	$x_k = \frac{1 \pm 1i}{4}, \frac{-1 \pm 1i}{4}$
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.	$P_6(x) = x^2 - \frac{1}{4}$	$x_k = \frac{1}{2}, -\frac{1}{2}$



**Fig. 7 (continued to next page).** 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.



**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.

## 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. CONFLICT OF INTEREST

The authors declare no conflict of interest.

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