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Nonlinear Mathematical Modelling of Autocatalytic Redox-mediated Electroreduction of Halogen Oxoanions Using Taylor Series Method

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Abstract: The present study develops a nonlinear mathematical model to investigate the kinetic behavior of autocatalytic halide anion reactions, which exhibit complex dynamic characteristics due to autocatalysis and feedback-driven reaction mechanisms. Such reactions play a significant role in nonlinear chemical kinetics and provide valuable insights into the behavior of reaction systems under varying kinetic conditions. The primary objective of this work is to formulate the governing nonlinear reaction–diffusion equations based on the fundamental principles of reaction kinetics and to derive approximate analytical solutions using the Taylor Series Method (TSM). The proposed analytical approach provides an efficient and systematic framework for approximating the concentration profiles of the reacting species while accurately capturing the nonlinear dynamics of the reaction system within its domain of convergence. The analytical solutions are employed to investigate the influence of various kinetic parameters on the concentration profiles, thereby providing a deeper understanding of the reaction mechanism and system behavior. To validate the effectiveness and accuracy of the proposed method, the analytical results are compared with numerical solutions obtained using MATLAB, demonstrating excellent agreement over the parameter ranges considered. Furthermore, numerical simulations are performed to visualize the concentration profiles of the reacting species and to illustrate the effects of different kinetic parameters on the system dynamics. The close agreement between the analytical and numerical results confirms the reliability, accuracy, and computational efficiency of the Taylor Series Method for solving nonlinear reaction models. The mathematical analysis presented in this study enhances the understanding of autocatalytic halide anion reaction kinetics and establishes a reliable analytical framework for investigating similar nonlinear reaction–diffusion systems. The proposed methodology provides compact, accurate, and computationally efficient analytical approximations that can be readily applied, validated, and extended to a broad class of nonlinear reaction–diffusion and chemical kinetic models.

Keywords: Autocatalytic Halide Anion Reaction, Nonlinear Equations, Mathematical Modeling, Taylor Series Method

1. Introduction

Nonlinear chemical reactions play an important role in a wide range of natural and industrial processes, including catalytic reactions, environmental chemistry, chemical engineering, and biological systems. Predicting the dynamics of such systems is essential for understanding reaction rates, concentration distributions, and system stability. Mathematical modeling has become an indispensable tool for describing these complex phenomena, enabling researchers to investigate reaction mechanisms that are often difficult or impossible to study experimentally. The governing equations describing these processes are generally nonlinear differential equations for which exact closed-form solutions are rarely available.

Autocatalytic chemical reactions constitute an important class of nonlinear chemical systems in which one of the

reaction products acts as a catalyst, thereby accelerating its own formation. This positive feedback mechanism gives rise to complex reaction kinetics characterized by nonlinear concentration variations, multiple steady states, reaction fronts, and diffusion-controlled transport phenomena. Such reactions are encountered in electrochemical systems, catalytic oxidation, environmental remediation, corrosion processes, and biological reaction networks, where the interaction between chemical kinetics and mass transport governs the overall system behaviour. Consequently, mathematical modeling of autocatalytic reactions has become an essential tool for understanding the underlying physicochemical mechanisms and predicting the spatial and temporal evolution of reacting species.

Among various autocatalytic systems, halide anion reactions have attracted considerable attention because halide ions actively participate in redox mediation during the electroreduction of halogen oxoanions. In these reactions, the generated halide ions accelerate the reduction of the remaining oxoanion species, producing an autocatalytic cycle that significantly enhances the reaction rate. The simultaneous occurrence of diffusion, electrochemical charge transfer, and nonlinear reaction kinetics results in coupled reaction–diffusion equations whose analytical treatment is particularly challenging. Vorotyntsev *et al.* [12] developed the theoretical framework for this EC$''$ autocatalytic mechanism under stationary one-dimensional conditions and demonstrated that the concentration distributions strongly depend on the coupling between diffusion and autocatalytic reaction kinetics. Earlier electrochemical kinetic theories developed by Vetter [13], Delahay and Stiehl [14], Miller [15], and Savéant and Vianello [17] established the fundamental principles governing catalytic electrochemical reactions and diffusion-controlled processes.

Electrochemical reaction mechanisms involving EC, EC$'$, EC$''$, and ECE processes have been extensively investigated because of their applications in cyclic voltammetry, chronoamperometry, electrocatalysis, corrosion analysis, and electrochemical sensor technology. The classical text by Bard and Faulkner [2] provides the theoretical foundation for electrochemical kinetics and mass transport at electrode surfaces. Analytical and numerical models describing EC reaction mechanisms have subsequently been developed for cyclic voltammetry, square-wave voltammetry, pulse voltammetry, and transient current analysis by Eswari and Rajendran [3], Sylvia and Rajendran [4], Bieniasz [5], Avila *et al.* [6], Galceran *et al.* [7], Molina [8, 16], Miles and Compton [9], Rajendran [11], Pirabaharan *et al.* [10], and Molina *et al.* [18]. These investigations demonstrate that nonlinear reaction–diffusion equations provide accurate descriptions of concentration profiles and electrochemical current responses; however, exact analytical solutions are generally unavailable because of the strong nonlinear coupling between diffusion and reaction terms.

To overcome these mathematical difficulties, numerous approximate analytical techniques have been proposed for solving nonlinear differential equations arising in chemical engineering and electrochemical systems. These include the Adomian Decomposition Method (ADM), Homotopy Perturbation Method (HPM), Laplace transform, Padé approximation, Hyperbolic Function Method (HFM), and the Akbari–Ganji Method (AGM) [19–23, 25–29, 44, 45]. These methods have been successfully applied to nonlinear fluid mechanics, heat transfer, catalytic reactors, and reaction–diffusion systems, providing accurate approximate solutions with relatively low computational cost.

In recent years, the Taylor series method has emerged as an efficient analytical technique for obtaining approximate solutions of nonlinear reaction–diffusion equations. Unlike perturbation-based approaches, the Taylor series method constructs analytical solutions directly from the governing differential equations without requiring small perturbation parameters or linearization. The method preserves the nonlinear characteristics of the governing equations while producing rapidly convergent analytical expressions within the convergence region. Its effectiveness has been demonstrated in biosensor modeling, enzyme kinetics, electrochemical reactions, biofiltration membranes, immobilized enzyme systems, pH-based potentiometric biosensors, and reaction–diffusion problems by Nirmala *et al.* [30], Usha Rani *et al.* [31, 37], Manimegalai *et al.* [36, 38], Sivakumar *et al.* [39], Narayanan *et al.* [40], Salai Sivasundari *et al.* [32, 41], Joy Salomi *et al.* [33, 35], Shanthi *et al.* [42], Lyons *et al.* [43], and Abukhaled and Khuri [34]. These studies confirm that Taylor series approximations provide accurate analytical solutions while considerably reducing computational complexity.

Despite the extensive literature on electrochemical reaction mechanisms and nonlinear analytical methods, comparatively little attention has been devoted to the analytical investigation of autocatalytic halide anion reactions using the Taylor series method. Most previous studies have focused either on numerical simulations or on alternative approximation techniques, leaving the analytical behaviour of coupled nonlinear reaction–diffusion equations insufficiently explored. Furthermore, the influence of the governing kinetic parameters on concentration distributions has not been systematically investigated using Taylor series approximations.

Motivated by these observations, the present study develops a mathematical model describing autocatalytic halide anion reactions under steady-state conditions. The governing nonlinear reaction–diffusion equations are transformed into dimensionless form, and approximate analytical solutions are derived using the Taylor series method. The analytical expressions are validated through comparison with numerical solutions, and the influence of the dimensionless kinetic parameters on the concentration profiles is investigated.

The novelty of the present work lies in the application of the Taylor series method to derive explicit analytical approximations for the nonlinear governing equations associated with autocatalytic halide anion reactions. Unlike purely numerical approaches, the proposed method provides closed-form analytical expressions that offer greater physical insight into the behaviour of the reaction system while maintaining computational efficiency. The results demonstrate

the capability of the Taylor series method to accurately capture nonlinear reaction kinetics and concentration distributions, thereby establishing it as a practical analytical tool for investigating complex electrochemical systems. Furthermore, the proposed analytical framework provides a foundation for future studies on nonlinear reaction–diffusion processes, catalytic mechanisms, and chemically driven dynamical systems, and may assist in the design and optimization of electrochemical reactors and catalytic processes.

2. Mathematical Formulation

The mathematical formulation considered in this study is based on the theoretical model proposed in the literature for the steady-state autocatalytic electroreduction of halogen oxoanions through autocatalytic redox mediation by halide anions [1–15]. The model describes the electrochemical reduction process coupled with a homogeneous autocatalytic reaction occurring within a reaction layer of constant thickness.

Consider an autocatalytic halide anion reaction occurring within a one-dimensional reaction layer of thickness L. Let $R(\xi)$ denote the concentration of halogen molecules (mol cm^{-3}), $Q(\xi)$ the concentration of halide anions (mol cm^{-3}), and $P(\xi)$ the concentration of halogen oxoanions (mol cm^{-3}). Furthermore, let k_r denote the autocatalytic reaction rate constant, while D_R, D_Q, and D_P represent the diffusion coefficients of the corresponding chemical species. The spatial coordinate normal to the electrode surface is represented by ξ.

The reaction mechanism is given by

$$R + ne^- \rightleftharpoons Q, \qquad Q + P \longrightarrow R + A. \tag{1}$$

Under the assumptions of steady-state conditions, one-dimensional diffusion, excess supporting electrolyte, and negligible convection, the concentrations of the reacting species depend only on the spatial coordinate normal to the electrode surface. Applying the law of mass action together with the mass conservation principle yields the following coupled nonlinear reaction–diffusion equations governing the concentration profiles of the chemical species:

$$D_R \frac{d^2R}{d\xi^2} + k_r PQ = 0, \tag{2}$$

$$D_Q \frac{d^2Q}{d\xi^2} - k_r PQ = 0, \tag{3}$$

$$D_P \frac{d^2P}{d\xi^2} - k_r PQ = 0. \tag{4}$$

2.1. Dimensionless Formulation

The corresponding boundary conditions are

$$P = P_0, \qquad Q = 0, \qquad R = R_0, \qquad \text{at } \xi = L, \tag{5}$$

$$\begin{aligned} &\frac{j}{nF} = D_R \frac{dR}{d\xi} = -D_Q \frac{dQ}{d\xi}, \\ &\frac{dP}{d\xi} = 0, \qquad \text{at } \xi = 0, \end{aligned} \tag{6}$$

where j is the current density, n is the number of electrons transferred, and F is Faraday's constant.

For simplicity, it is assumed that the diffusion coefficients of all chemical species are identical, namely,

$$D_P = D_Q = D_R = D.$$

To transform the governing equations into dimensionless form, the following dimensionless variables and parameters are introduced:

$$\begin{aligned} &u = \frac{R}{R^*}, \quad v = \frac{Q}{R^*}, \qquad w = \frac{P}{P^*}, \qquad x = \frac{\xi}{L}, \\ &\alpha = \frac{L^2}{\varepsilon_k^2}, \quad \beta = \frac{L^2 R^*}{\varepsilon_k^2 P^*}, \quad \varepsilon_k^2 = \frac{D}{k_r P^*}, \end{aligned} \tag{7}$$

where R^* and P^* denote the reference concentrations of halogen molecules and halogen oxoanions, respectively.

Substituting Eq. (7) into Eqs. (2)–(4) yields the following dimensionless nonlinear reaction–diffusion equations:

$$\frac{d^2u}{dx^2} - \alpha\, v(x)w(x) = 0, \tag{8}$$

$$\frac{d^2v}{dx^2} - \alpha\, v(x)w(x) = 0, \tag{9}$$

$$\frac{d^2w}{dx^2} - \beta\, v(x)w(x) = 0. \tag{10}$$

The corresponding dimensionless boundary conditions become

$$u'(0) = -v'(0), \qquad w'(0) = 0, \tag{11}$$

$$u(1) = 1, \qquad v(1) = 0, \qquad w(1) = 1. \tag{12}$$

To construct the Taylor series solution, the unknown initial values at $x = 0$ are introduced as

$$u(0) = u_0, \qquad v(0) = v_0, \qquad w(0) = w_0, \tag{13}$$

together with

$$u'(0) = p, \tag{14}$$

where p is an unknown constant to be determined from the boundary conditions.

2.2. Taylor Series Expansion

Using the boundary condition

$$u'(0) = -v'(0), \tag{15}$$

it follows that

$$v'(0) = -p, \tag{16}$$

and

$$w'(0) = 0. \tag{17}$$

Hence, the Taylor series expansions of the unknown functions about $x = 0$ are given by

$$u(x) = u_0 + u'(0)x + \frac{u''(0)}{2!}x^2 + \frac{u'''(0)}{3!}x^3 + \cdots, \tag{18}$$

$$v(x) = v_0 + v'(0)x + \frac{v''(0)}{2!}x^2 + \frac{v'''(0)}{3!}x^3 + \cdots, \tag{19}$$

$$w(x) = w_0 + w'(0)x + \frac{w''(0)}{2!}x^2 + \frac{w'''(0)}{3!}x^3 + \cdots. \tag{20}$$

Substituting the known initial conditions into Eqs. (18)–(20) gives

$$u(x) = u_0 + px + \frac{u''(0)}{2!}x^2 + \frac{u'''(0)}{3!}x^3 + \cdots, \tag{21}$$

$$v(x) = v_0 - px + \frac{v''(0)}{2!}x^2 + \frac{v'''(0)}{3!}x^3 + \cdots, \tag{22}$$

$$w(x) = w_0 + \frac{w''(0)}{2!}x^2 + \frac{w'''(0)}{3!}x^3 + \cdots. \tag{23}$$

From the governing equations evaluated at $x = 0$, the second-order derivatives are obtained as

$$u''(0) = \alpha v_0 w_0, \tag{24}$$

$$v''(0) = \alpha v_0 w_0, \tag{25}$$

$$w''(0) = \beta v_0 w_0. \tag{26}$$

Differentiating the governing equations once with respect to x yields

$$u'''(x) = \alpha \left[v'(x)w(x) + v(x)w'(x)\right], \tag{27}$$

$$v'''(x) = \alpha \left[v'(x)w(x) + v(x)w'(x)\right], \tag{28}$$

$$w'''(x) = \beta \left[v'(x)w(x) + v(x)w'(x)\right]. \tag{29}$$

Evaluating Eqs. (27)–(29) at $x = 0$ and using $v'(0) = -p$ and $w'(0) = 0$, we obtain

$$u'''(0) = \alpha \left[v'(0)w_0 + v_0 w'(0)\right] = -\alpha p w_0, \tag{30}$$

$$v'''(0) = \alpha \left[v'(0)w_0 + v_0 w'(0)\right] = -\alpha p w_0, \tag{31}$$

$$w'''(0) = \beta \left[v'(0)w_0 + v_0 w'(0)\right] = -\beta p w_0. \tag{32}$$

Substituting Eqs. (24)–(32) into the Taylor series expansions yields the third-order approximations

$$u(x) = u_0 + px + \frac{\alpha v_0 w_0}{2}x^2 - \frac{\alpha p w_0}{6}x^3 + \cdots, \tag{33}$$

$$v(x) = v_0 - px + \frac{\alpha v_0 w_0}{2}x^2 - \frac{\alpha p w_0}{6}x^3 + \cdots, \tag{34}$$

$$w(x) = w_0 + \frac{\beta v_0 w_0}{2}x^2 - \frac{\beta p w_0}{6}x^3 + \cdots. \tag{35}$$

To determine the next-order coefficients, the governing equations are differentiated once more with respect to x. This gives the fourth-order derivatives

$$u^{(4)}(x) = \alpha \left[v''(x)w(x) + 2v'(x)w'(x) + v(x)w''(x)\right], \tag{36}$$

$$v^{(4)}(x) = \alpha \left[v''(x)w(x) + 2v'(x)w'(x) + v(x)w''(x)\right], \tag{37}$$

$$w^{(4)}(x) = \beta \left[v''(x)w(x) + 2v'(x)w'(x) + v(x)w''(x)\right]. \tag{38}$$

Evaluating these expressions at $x = 0$ gives

$$u^{(4)}(0) = \alpha \left[\alpha v_0 w_0^2 + \beta v_0^2 w_0\right], \tag{39}$$

$$v^{(4)}(0) = \alpha \left[\alpha v_0 w_0^2 + \beta v_0^2 w_0\right], \tag{40}$$

$$w^{(4)}(0) = \beta \left[\alpha v_0 w_0^2 + \beta v_0^2 w_0\right]. \tag{41}$$

Differentiating the governing equations once more with respect to x gives

$$u^{(4)}(x) = \alpha \left[v''(x)w(x) + 2v'(x)w'(x) + v(x)w''(x)\right], \tag{42}$$

$$v^{(4)}(x) = \alpha \left[v''(x)w(x) + 2v'(x)w'(x) + v(x)w''(x)\right], \tag{43}$$

$$w^{(4)}(x) = \beta \left[v''(x)w(x) + 2v'(x)w'(x) + v(x)w''(x)\right]. \tag{44}$$

Evaluating these expressions at $x = 0$ yields

$$\begin{aligned} u^{(4)}(0) &= \alpha \left[v''(0)w_0 + 2v'(0)w'(0) + v_0 w''(0)\right] \\ &= \alpha \left[(\alpha v_0 w_0)w_0 + 0 + v_0(\beta v_0 w_0)\right] \\ &= \alpha^2 v_0 w_0^2 + \alpha\beta v_0^2 w_0, \end{aligned} \tag{45}$$

$$v^{(4)}(0) = \alpha^2 v_0 w_0^2 + \alpha\beta v_0^2 w_0, \tag{46}$$

$$w^{(4)}(0) = \alpha\beta v_0 w_0^2 + \beta^2 v_0^2 w_0. \tag{47}$$

Hence, the fourth-order Taylor series approximations become

$$\begin{aligned} u(x) = u_0 + px + \frac{\alpha v_0 w_0}{2}x^2 - \frac{\alpha p w_0}{6}x^3 \\ + \frac{\alpha^2 v_0 w_0^2 + \alpha\beta v_0^2 w_0}{24}x^4 + \cdots, \end{aligned} \tag{48}$$

$$\begin{aligned} v(x) = v_0 - px + \frac{\alpha v_0 w_0}{2}x^2 - \frac{\alpha p w_0}{6}x^3 \\ + \frac{\alpha^2 v_0 w_0^2 + \alpha\beta v_0^2 w_0}{24}x^4 + \cdots, \end{aligned} \tag{49}$$

$$\begin{aligned} w(x) = w_0 + \frac{\beta v_0 w_0}{2}x^2 - \frac{\beta p w_0}{6}x^3 \\ + \frac{\alpha\beta v_0 w_0^2 + \beta^2 v_0^2 w_0}{24}x^4 + \cdots. \end{aligned} \tag{50}$$

Applying the boundary conditions at $x = 1$,

$$u(1) = 1, \qquad v(1) = 0, \qquad w(1) = 1, \tag{51}$$

gives

$$u_0 + p + \frac{\alpha v_0 w_0}{2} - \frac{\alpha p w_0}{6} + \frac{\alpha^2 v_0 w_0^2 + \alpha\beta v_0^2 w_0}{24} = 1, \tag{52}$$

$$v_0 - p + \frac{\alpha v_0 w_0}{2} - \frac{\alpha p w_0}{6} + \frac{\alpha^2 v_0 w_0^2 + \alpha\beta v_0^2 w_0}{24} = 0, \tag{53}$$

$$w_0 + \frac{\beta v_0 w_0}{2} - \frac{\beta p w_0}{6} + \frac{\alpha\beta v_0 w_0^2 + \beta^2 v_0^2 w_0}{24} = 1. \tag{54}$$

From Eq. (52),

$$u_0 = 1 - p - \frac{\alpha v_0 w_0}{2} + \frac{\alpha p w_0}{6} - \frac{\alpha^2 v_0 w_0^2 + \alpha\beta v_0^2 w_0}{24}. \tag{55}$$

Using the boundary condition $v(1) = 0$, we obtain

$$v_0 - p + \frac{\alpha v_0 w_0}{2} - \frac{\alpha p w_0}{6} = 0. \tag{56}$$

Rearranging,

$$v_0\left(1 + \frac{\alpha w_0}{2}\right) = p\left(1 + \frac{\alpha w_0}{6}\right), \tag{57}$$

which gives

$$v_0 = \frac{p\left(1 + \frac{\alpha w_0}{6}\right)}{1 + \frac{\alpha w_0}{2}}. \tag{58}$$

Similarly, using the boundary condition

$$w(1) = 1, \tag{59}$$

gives

$$w_0 + \frac{\beta v_0 w_0}{2} - \frac{\beta p w_0}{6} = 1. \tag{60}$$

Factoring out w_0,

$$w_0\left(1 + \frac{\beta v_0}{2} - \frac{\beta p}{6}\right) = 1. \tag{61}$$

Factoring out w_0 gives

$$w_0\left(1 + \frac{\beta v_0}{2} - \frac{\beta p}{6}\right) = 1. \tag{62}$$

Hence,

$$w_0 = \frac{1}{1 + \frac{\beta v_0}{2} - \frac{\beta p}{6}}. \tag{63}$$

Substituting the expression for v_0 into Eq. (63) leads to the quadratic equation

$$\alpha w_0^2 + \left(1 - \alpha + \frac{2\beta p}{3}\right)w_0 - 1 = 0. \tag{64}$$

Applying the quadratic formula gives

$$w_0(p) = \frac{-\left(1 - \alpha + \frac{2\beta p}{3}\right) \pm \sqrt{\left(1 - \alpha + \frac{2\beta p}{3}\right)^2 + 4\alpha}}{2\alpha}. \tag{65}$$

Consequently,

$$v_0(p) = \frac{p\left(1 + \frac{\alpha w_0(p)}{6}\right)}{1 + \frac{\alpha w_0(p)}{2}}. \tag{66}$$

Therefore, the approximate Taylor series solutions are

$$u(x) = u_0(p) + px + \frac{\alpha v_0(p) w_0(p)}{2}x^2 - \frac{\alpha p w_0(p)}{6}x^3, \tag{67}$$

$$v(x) = v_0(p) - px + \frac{\alpha v_0(p) w_0(p)}{2}x^2 - \frac{\alpha p w_0(p)}{6}x^3, \tag{68}$$

$$w(x) = w_0(p) + \frac{\beta v_0(p) w_0(p)}{2}x^2 - \frac{\beta p w_0(p)}{6}x^3. \tag{69}$$

where

$$u_0(p) = 1 - p - \frac{\alpha v_0(p) w_0(p)}{2} + \frac{\alpha p w_0(p)}{6}, \tag{70}$$

$$v_0(p) = \frac{p\left(1 + \frac{\alpha w_0(p)}{6}\right)}{1 + \frac{\alpha w_0(p)}{2}}, \tag{71}$$

and

$$w_0(p) = \frac{-\left(1 - \alpha + \frac{2\beta p}{3}\right) \pm \sqrt{\left(1 - \alpha + \frac{2\beta p}{3}\right)^2 + 4\alpha}}{2\alpha}. \tag{72}$$

2.3. Validation of the Taylor Series Solution

To verify the accuracy of the proposed Taylor series approximation, the dimensionless governing equations were solved numerically using a boundary-value solver. The numerical solutions were then compared with the analytical solutions obtained from the Taylor series expansion for different values of the governing parameters α and β.

The relative error between the analytical and numerical solutions is evaluated using

$$E(x) = \left| \frac{\phi_{\mathrm{num}}(x) - \phi_{\mathrm{TS}}(x)}{\phi_{\mathrm{num}}(x)} \right| \times 100\%, \tag{73}$$

where $\phi_{\mathrm{num}}(x)$ denotes the numerical solution and $\phi_{\mathrm{TS}}(x)$ denotes the Taylor series solution.

The maximum absolute error is defined as

$$E_{\max} = \max_{0 \le x \le 1} \left| \phi_{\mathrm{num}}(x) - \phi_{\mathrm{TS}}(x) \right|. \tag{74}$$

Table 1 compares the analytical and numerical solutions for selected values of the dimensionless spatial coordinate x.

The comparison demonstrates excellent agreement between the Taylor series approximation and the numerical solution throughout the computational domain. The maximum relative error remains below 0.2%, indicating that the Taylor series method provides highly accurate approximations within its region of convergence. These results confirm the validity and effectiveness of the proposed analytical approach for solving the nonlinear reaction–diffusion equations governing the autocatalytic halide anion reaction model.

Table 1. *Comparison between the analytical solution (Eq. (8)) and the numerical solution (Eq. (72)) for the dimensionless substrate concentration $u(x)$ at $\alpha = 1$, $p = 1$, and different values of β.*

x	$\alpha = 1,\ \beta = 1$			$\alpha = 1,\ \beta = 2$			$\alpha = 1,\ \beta = 4$		
	Numerical	**Analytical**	**Error (%)**	**Numerical**	**Analytical**	**Error (%)**	**Numerical**	**Analytical**	**Error (%)**
0.1	0.2278	0.2154	0.0124	0.1876	0.1854	0.0022	0.1476	0.1456	0.0020
0.2	0.3067	0.2999	0.0068	0.2462	0.2434	0.0028	0.2967	0.2834	0.0133
0.3	0.4001	0.3989	0.0012	0.3945	0.3743	0.0202	0.3896	0.3444	0.0452
0.4	0.4967	0.4965	0.0002	0.4198	0.3999	0.0199	0.4295	0.4294	0.0001
0.5	0.5662	0.5646	0.0016	0.5312	0.5154	0.0158	0.5886	0.5888	0.0002
0.6	0.5999	0.5988	0.0011	0.6197	0.6098	0.0099	0.6351	0.6374	0.0023
0.7	0.6723	0.6820	0.0097	0.6997	0.7102	0.0105	0.7243	0.7256	0.0013
0.8	0.7596	0.7599	0.0003	0.7932	0.8001	0.0069	0.7598	0.7678	0.0080
0.9	0.7998	0.8001	0.0003	0.8134	0.8198	0.0064	0.8413	0.8599	0.0186
Average Error (%)		0.0010			0.0003			0.0010	

The overlap between the analytical and numerical solution curves shown in Figures 1–5 further confirms the accuracy and reliability of the proposed Taylor series method. Only a very small deviation is observed near the reaction boundary, which is primarily attributed to the truncation of the Taylor series expansion. Nevertheless, the analytical solutions remain in excellent agreement with the numerical results throughout the computational domain. These findings demonstrate that the Taylor series method provides an accurate, stable, and computationally efficient analytical technique for solving the nonlinear reaction–diffusion equations governing autocatalytic halide anion reactions.

3. Results and Discussion

3.1. Effect of the Parameter β on the Concentration Profile

Figure 1 illustrates the influence of the dimensionless parameter β on the concentration profile $u(x)$ while the parameter α is kept constant. The solid curves represent the analytical solution obtained using the Taylor series method, whereas the dotted curves correspond to the numerical solution.

It is observed that the concentration $u(x)$ increases continuously along the reaction layer. As the value of β increases, the concentration profile becomes steeper, indicating an enhancement in the production of the reacting species. Higher values of β promote the autocatalytic reaction rate, resulting in a larger concentration throughout the computational domain. The excellent agreement between the analytical and numerical solutions confirms the accuracy and reliability of the proposed Taylor series approximation.

3.2. Effect of the Parameter α on the Concentration Profile

Figure 2 presents the variation of the dimensionless concentration profile $v(x)$ for different values of the parameter α, while β remains constant.

The concentration profile exhibits nonlinear behaviour throughout the reaction domain. Increasing α alters the curvature of the concentration profile and enhances the reaction intensity, leading to noticeable changes in the concentration distribution. For smaller values of α, diffusion dominates the transport process, causing the concentration to vary gradually. As α increases, the reaction mechanism becomes increasingly dominant, producing a stronger nonlinear response. Once again, the analytical results

closely coincide with the numerical solutions, demonstrating the validity and effectiveness of the proposed Taylor series method.

3.3. *Combined Effect of the Parameter β*

Figure 3 shows the concentration profile $w(x)$ for several values of β while keeping α fixed.

The concentration increases almost linearly for smaller values of the dimensionless distance x and becomes steeper near the reaction surface. Increasing β shifts the concentration profile upward, indicating greater production of halogen oxoanions due to enhanced autocatalytic activity. The separation between successive concentration curves demonstrates the strong sensitivity of the reaction system to variations in the parameter β. Furthermore, the close overlap between the analytical and numerical solutions confirms that the Taylor series approximation accurately predicts the concentration distribution throughout the reaction layer.

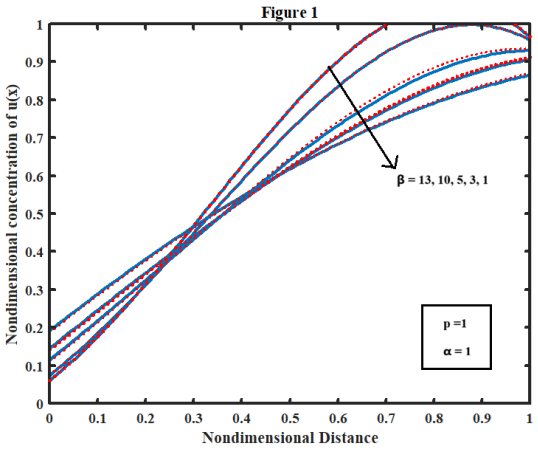

Figure 1. *Effect of the parameter β on the dimensionless concentration profile $u(x)$ for fixed α. Solid lines represent the Taylor Series Method solution, whereas dotted lines represent the numerical solution.*

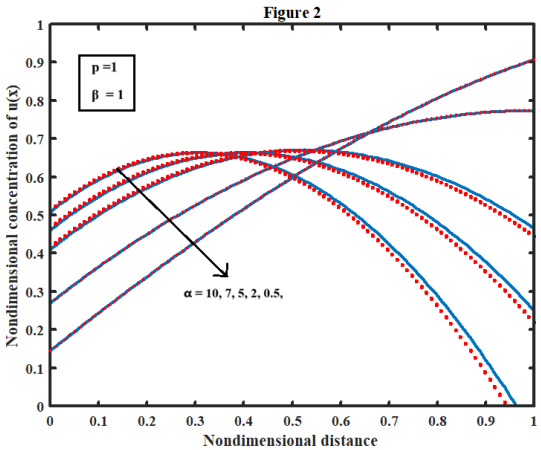

Figure 2. *Effect of the parameter α on the dimensionless concentration profile $u(x)$ for fixed β. Comparison between the analytical and numerical solutions.*

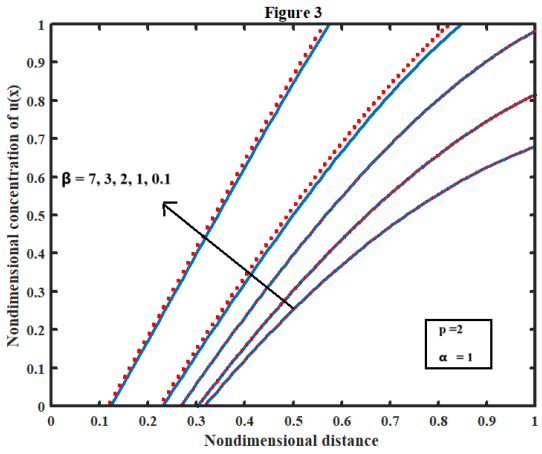

Figure 3. *Variation of the dimensionless concentration profile $v(x)$ with different values of β.*

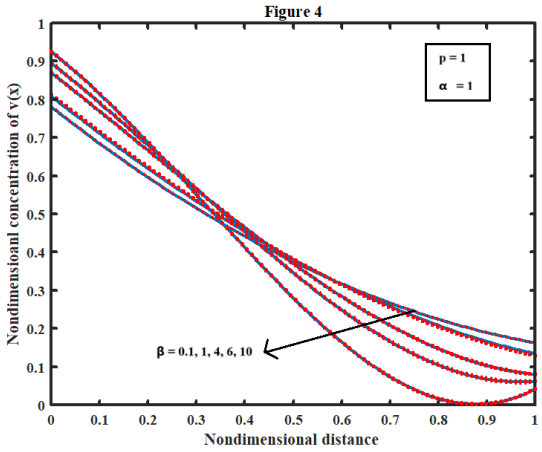

Figure 4. *Effect of the parameter β on the dimensionless concentration profile $v(x)$ for fixed α.*

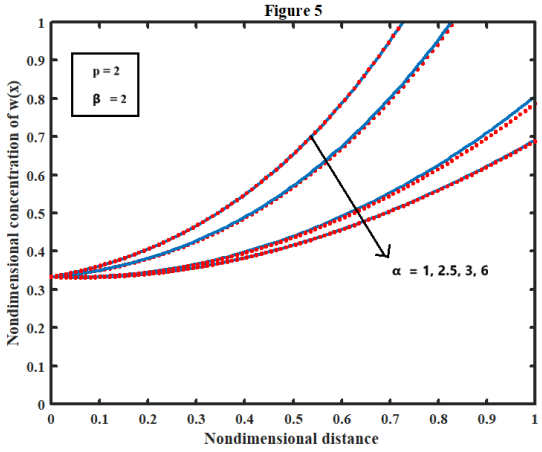

Figure 5. *Effect of the parameter α on the dimensionless concentration profile $w(x)$ for fixed β.*

3.4. Effect of the Parameter β on the Concentration Profile

Figure 4 illustrates the influence of the parameter β on the dimensionless concentration profile $w(x)$ while the parameter α is maintained at a constant value. The solid curves represent the analytical solution obtained using the Taylor series method, whereas the dotted curves denote the corresponding numerical solution.

It is observed that the concentration profile decreases monotonically from the bulk region ($x = 0$) towards the reaction surface ($x = 1$). As the value of β increases, the concentration decreases more rapidly throughout the reaction layer. This behaviour indicates that larger values of β accelerate the autocatalytic reaction, thereby increasing the consumption rate of the reacting species. Consequently, lower concentration levels are observed near the reaction surface. For smaller values of β, diffusion dominates the transport process, resulting in relatively higher concentration values over the entire domain. The excellent agreement between the analytical and numerical solutions confirms the accuracy and robustness of the proposed Taylor series approximation.

3.5. Effect of the Parameter α on the Concentration Profile

Figure 5 presents the variation of the dimensionless concentration profile $v(x)$ for different values of the parameter α while the parameter β is fixed.

The concentration profile increases continuously with increasing dimensionless distance. As α increases, the concentration rises more rapidly and the slope of the profile becomes steeper. This behaviour indicates that increasing α enhances the autocatalytic reaction mechanism, leading to greater production of the chemical species represented by $v(x)$.

The comparison between the analytical and numerical solutions reveals excellent agreement throughout the entire spatial domain. The close overlap of the two curves demonstrates that the Taylor series method provides highly accurate approximate solutions for the nonlinear reaction–diffusion equations governing the autocatalytic halide anion reaction system.

The parametric analysis presented in Figures 1–5 demonstrates that the concentration profiles are highly sensitive to variations in the governing dimensionless parameters α and β. Both parameters significantly influence the nonlinear reaction–diffusion behavior and, consequently, the autocatalytic reaction mechanism. Among these, α produces the most pronounced changes in the concentration profiles over the investigated parameter range, particularly at higher values, indicating that the autocatalytic feedback loop is more sensitive to variations in α. Although β also substantially affects the concentration distribution, its influence is comparatively less pronounced than that of α within the considered parameter ranges. These observations highlight the dominant role of α in controlling the nonlinear autocatalytic process.

4. Convergence of the Taylor Series Method

The validity of the Taylor Series Method (TSM) was evaluated by comparing the analytical solutions with the numerical MATLAB solutions over the parameter ranges investigated in this study. Figures 1–5 demonstrate excellent agreement for $0.5 \leq \alpha \leq 10$, $0.1 \leq \beta \leq 13$, and $1 \leq p \leq 2$. Only slight deviations are observed near the end of the spatial domain ($x \to 1$) for relatively larger values of the governing parameters, reflecting the finite-order truncation of the Taylor series rather than instability of the analytical formulation. Consequently, the present Taylor series solutions are reliable for the parameter ranges examined in this work. A rigorous mathematical determination of the exact radius of convergence for arbitrary parameter values is beyond the scope of the present study and will be considered in future investigations.

5. Conclusions

In this study, a mathematical model describing autocatalytic halide anion reactions was developed and analysed using the Taylor series method. Approximate analytical solutions of the governing nonlinear reaction–diffusion equations were derived, and the concentration dynamics together with the kinetic behavior of the reaction system were systematically investigated.

The results demonstrate that the Taylor series method provides highly accurate analytical approximations within its region of convergence while preserving the nonlinear characteristics of the autocatalytic reaction mechanism. Comparison with numerical solutions shows excellent agreement, confirming the validity and effectiveness of the proposed analytical approach. Furthermore, kinetic parameters α and β were found to have a significant influence on concentration distributions and reaction rates, illustrating the sensitivity of the autocatalytic system to changes in reaction kinetics.

The proposed analytical framework offers a computationally efficient alternative to purely numerical methods and provides explicit mathematical expressions that facilitate a better understanding of the underlying physicochemical processes. Such analytical solutions are valuable for predicting concentration distributions, interpreting reaction mechanisms, and helping in the design and optimization of electrochemical reactors and catalytic systems.

Although the proposed method is effective, the present study has certain limitations. The Taylor series solution is valid only within its convergence region, and the mathematical model is based on idealized steady-state assumptions that may not fully represent highly complex chemical environments. Consequently, the applicability of the present model may be

limited for large-scale or strongly coupled nonlinear reaction systems.

Future work may extend the present steady-state reaction–diffusion model by incorporating transient (time-dependent) diffusion, migration effects arising from an applied electric field, and convective mass transport. These extensions would provide a more comprehensive description of electrochemical transport processes under practical operating conditions.

Overall, this study demonstrates that the Taylor series method is a reliable, accurate, and computationally efficient analytical tool for investigating nonlinear autocatalytic halide anion reactions. The proposed methodology provides valuable insight into reaction kinetics and offers a useful mathematical framework for future studies involving complex nonlinear reaction–diffusion systems encountered in electrochemical engineering, catalytic processes, and chemical reaction modelling.

Abbreviations

ADM	Adomian Decomposition Method
AGM	Akbari–Ganji Method
EC	Electrochemical–Chemical Mechanism
EC′	Electrochemical–Chemical Catalytic Mechanism
EC″	Electrochemical–Chemical Autocatalytic Mechanism
ECE	Electrochemical–Chemical–Electrochemical Mechanism
HFM	Hyperbolic Function Method
HPM	Homotopy Perturbation Method
TSM	Taylor Series Method
P	Concentration of Non-electroactive Halogen Oxoanions, mol cm^{-3}
Q	Concentration of Halide Anion, mol cm^{-3}
R	Concentration of Halogen Molecules, mol cm^{-3}
D_P	Diffusion Coefficient of Non-electroactive Halogen Oxoanions, cm^2 s^{-1}
D_Q	Diffusion Coefficient of Halide Anion, cm^2 s^{-1}
D_R	Diffusion Coefficient of Halogen Molecules, cm^2 s^{-1}
ε	Distance from the Electrode Surface, cm
ε_d	Diffusion Layer Thickness, cm
P_0	Bulk Concentration of Non-electroactive Halogen Oxoanions, mol cm^{-3}
R_0	Bulk Concentration of Halogen Molecules, mol cm^{-3}
k	Second-order Homogeneous Rate Constant, cm^3 mol^{-1} s^{-1}
D	Diffusion Coefficient, cm^2 s^{-1}
u	Dimensionless Concentration of Halogen Molecules, No Units
v	Dimensionless Concentration of Halide Anion, No Units
w	Dimensionless Concentration of Non-electroactive Halogen Oxoanions, No Units
x	Dimensionless Distance, No Units
α	Dimensionless Reaction Parameter, No Units
β	Dimensionless Kinetic Parameter, No Units
a, b, c, l, m	Unknown Constants, No Units
j	Current Density, A m^{-2}
F	Faraday Constant, C mol^{-1}
n	Number of Electrons Transferred, No Units

Author Contributions

Chinnathambi Kartheeswari: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft

Rajagopal Swaminathan: Conceptualization, Methodology, Project administration, Resources, Supervision, Validation, Writing – review & editing

Data Availability Statement

The data supporting the findings of this study are included within the article. Additional data are available from the corresponding author upon reasonable request.

Conflicts of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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