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ORIGINAL PAPER

An Analytical Studies of the Reaction- Diffusion Systems of Chemical Reactions

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Abstract
Reaction–diffusion systems are seen in not only many fields of science but also social behaviorus. In this work, Schnakenberg, Brusselator and Lengyel–Epstein models are considered that are the best known the chemical reaction–diffusion models and are also seen in a large scale of applications in biological or biochemical processes. Due to its importance in science and applications, for the considered models, till now the numerical and approximate solutions are obtained whereas the exact solutions in the explicit form were not obtained literature to our knowledge. Our main aim is to fill this gap by revealing their exact solutions. To obtain the exact solutions, the ansatz-based methods are considered in a novel way. The obtained results have a major role in the literature so that the considered models are seen in a large scale of applications not only chemical but also biological or biochemical processes.

Keywords Schnakenberg model · Brusselator model · Lengyel–Epstein model · Exact solutions

Introduction

In the real life, both classical and fractional mathematical models are important to explain the processes [18–31]. The most used one is Reaction–diffusion systems that are used to model many physical, chemical, biological, environmental and even sociological processes [1]. In examining the chemical reaction–diffusion models, Schnakenberg, Brusselator and Lengyel–Epstein models are the most seen ones. These models are also known as Tuning-type models which have been used for generating patterns in both chemical and biological systems [1]. Additionally, these models are important to include modern thermodynamics analysis, so they are hypothetical sets of chemical reactions. As a result of this reactions cause limit cycle oscillations and propose a qualitative description of biochemical oscillators. Reaction–Diffusion equations occurred naturally in systems formed by the interaction of

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many components and are widely used to describe various biological, chemical and physical systems. The classical reaction–diffusion equation or alias self-diffusion equation is

$$\frac{\partial u}{\partial t} = D\nabla^2 u + R(u) \tag{1}$$

where $u = u(x, t)$ represents density/concentration of a substance, D is the diffusion coefficient, $\nabla^2 u$ and $R(u)$ are the diffusion and the reaction terms, respectively [2]. The general two-component system is given by the following system;

$$\begin{cases} u_t = D_u \nabla^2 u + F(u, v) \\ v_t = D_v \nabla^2 v + G(u, v) \end{cases} \tag{2}$$

where D_u and D_v are the diffusion coefficients, $F(u, v)$ and $G(u, v)$ are the reaction terms. Additionally, two-component systems (Eq. (2)) are more useful than one-component i.e. reaction–diffusion equation (Eq. (1)) so, it is modified for a much larger range of possible phenomena.

In examining the chemical reaction–diffusion models, firstly Schnakenberg model [3] is a two-species model for trimolecular reactions.

$A \rightleftharpoons U$, $B \to V$, $2U + V \to 3U$.

The model, constructed by the law of mass action, is given by the following system;

$$\begin{cases} u_t - D_u \nabla^2 u = \alpha - u + u^2 v \\ v_t - D_v \nabla^2 v = \beta - u^2 v \end{cases} \tag{3}$$

where $u = u(x, t)$ and $v = v(x, t)$ represents concentration, D_u and D_v are the diffusion coefficients of the chemicals U and V, respectively. α and β are constants and represent the concentration of the A and B, the right sides of each equation of Eq. (3) are reaction terms. Although Eq. (3) is the model of the chemical process, it is used to model the spatial distribution of a morphogen in biology [4].

If there are four chemical reactions.

$A \to U$, $B + U \to V + D$, $2U + V \to 3U$, $U \to E$,

the corresponding model is known as Brusselator model that is generally given as

$$\begin{cases} u_t - D_u \nabla^2 u = \alpha - (\beta + 1)u + f(u)v \\ v_t - D_v \nabla^2 v = \beta u - f(u)v \end{cases} \tag{4}$$

where D_u and D_v are the diffusion coefficients and $u = u(x, t)$ and $v = v(x, t)$ represents concentration of the chemicals U and V, respectively. α and β are positive fixed concentration of the A and B, and right sides of each equation of Eq. (4) are reaction terms that $f(u)$ is a nonnegative and nondecreasing function. When $f(u) = u^2$, the existence of a global solution to Eq. (4) was obtained by Rothe [1, 5]. For more general nonlinearities $f(u)$, the existence of global solution to Eq. (4) is given by the assumption $D_u = D_v$[1].

Equation (3) and Eq. (4) are derived from simple reactions where an autocatalytic process is present, the only difference between them is how many chemical reactions occur in the process [1, 6].

Lengyel–Epstein model corresponds a special reaction that is the chlorite–iodide–malonic acid and starch reaction (CIMA) in an open unstirred gel reactor [1, 7]. It is reaction scheme is given as.

$$\begin{cases} MA + I_2 \rightarrow IMA + I^- + H^+ \\ ClO_2 + I^- \rightarrow \frac{1}{2} I_2 + ClO_2^- \\ ClO_2^- + 4I^- + 4H^+ \rightarrow Cl^- + 2I_2 + 2H_2O \end{cases}.$$

As it is seen reaction scheme, different from first two models, there are five reactants. But the model is established on the time evolution of the concentrations of $\left[I^-\right]$ and $\left[ClO_2^-\right]$ which are represented by $u = u(x,t)$ and $v = v(x,t)$, respectively [7]. Lengyel–Epstein model is given by Eq. (5):

$$\begin{cases} u_t - \nabla^2 u = \alpha - u - \dfrac{4uv}{1+u^2} \\ v_t - d\nabla^2 v = \beta\left(u - \dfrac{uv}{1+u^2}\right) \end{cases} \tag{5}$$

where α,$\beta > 0$ are rate constants that dependent on feed concentrations, d is the diffusion coefficient and the right sides of each equation of Eq. (5) are reaction terms.

The models taken into consideration have been extensively investigated both analytically and numerically in recent years [1, 8–10]. In addition, homotopy perturbation method, homotopy analysis method and Adomian decomposition method are considered to obtain approximate solutions of the models [4, 11, 12]. But, the exact solutions of the considered models were not obtained in the explicit form in the literature to our knowledge. Therefore, our main aim is to fill this gap by revealing their exact solutions. The exact solutions will be obtained via combination of Bernoulli approximation method and Hermite approximation method [15–17]. Each method is the modification of the well-known auxiliary equation method. Applying the combination of methods has been the first time in the literature. The obtained results have a major role in the literature so that the considered models are seen in a large scale of applications both in chemistry and biology. Additionally, the costs can be reduced by using the obtained results.

Briefly, the exact solutions of the considered chemical models are not seen in the literature to our knowledge. Most of the works in the literature include experimental and numerical solutions. By means of novel methodology, the exact solutions of the models will be given in the explicit form. This is advantage for the interpretation of diffusion coefficients or feed concentrations. In the following parts, firstly the brief of the considered methodology is given and then, the exact solutions are proposed for each model.

Methodology

For the system, the combination of Bernoulli approximation method [15] and Hermite approximation method [17], each of the methods are seen as a modification of the well-known auxiliary equation method [13, 16].

$P_i\left(x, y, t, u_i, (u_i)_x, (u_i)_t, (u_i)_{xx}, (u_i)_{xt}, (u_i)_{tt}, ...\right)$, $i = 1, 2, ...$ nonlinear partial differential system (NPDS) is considered and reduced by using the wave transformation $\xi = x + \mu y - ct$, $c \neq 0$, $\mu \neq 0$ into the nonlinear ordinary differential system N_i $\left(\xi, u_i, u_i', u_i'', u_i''', ...\right)$, $i = 1, 2, ...$ The obtained solutions are invariant with respect to translation in space. The ansatzes are assumed to be as finite sum of the solution of the auxiliary equations $u_i(\xi) = \sum_{j=0}^{M_i} a_{ij} z(\xi)^j$, $(i = 1, 2, ..)$ where M_i is determined via balancing principle [14] for each equation in the system and a_{ij} are unknown parameters which are determined as a result of nonlinear algebraic system. In this work,

- The classical Bernoulli differential equation $\frac{dz(\xi)}{d\xi} = Pz(\xi) + Qz^k(\xi)$ where P and Q are parameters, which will be determined as a solution of nonlinear algebraic system, and $k > 1$ is an integer. Its solution is $z(\xi) = \frac{P\exp(P\xi)}{-Q\exp(P\xi)+PC_3}$ for $k = 2$ and C_3 is an integration constant.
- Hermite differential equation $\frac{d^2\omega}{d\zeta^2} = 2\zeta\left(\frac{d\omega}{d\zeta}\right) + \lambda\omega(\zeta) = 0$ and its solution is

$$\omega(\xi) = C_1 KummerM\left(\frac{1}{2} + \frac{\lambda}{4}, \frac{3}{2}, \xi^2\right)\xi + C_2 KummerU\left(\frac{1}{2} + \frac{\lambda}{4}, \frac{3}{2}, \xi^2\right)\xi$$

where C_1 and C_2 are integration constants, are considered as the auxiliary equations.

Results and Discussion

In this section, the models taken into consideration are solved via the new approach which is a combination of two well-known methods. The analytical solutions in the explicit form were not obtained literature to our knowledge; these solutions will be the first in the literature. Our main aim is to fill this gap by revealing their exact solutions.

The Schnakenberg Model

The Schnakenberg model that is generally given as

$$\begin{cases} u_t = D_u\nabla^2 u + \alpha - u + u^2 v \\ v_t = D_v\nabla^2 v + \beta - u^2 v \end{cases} \tag{6}$$

where D_u and D_v are the diffusion coefficients of the chemicals U and V, respectively. α and β are constants and represent the concentration of the A and B.

Using the wave transformation $\xi = x + \mu y - ct$, $c \neq 0$, $\mu \neq 0$, the system is reduced into the following system;

$$\begin{cases} -cu' - D_u\left(1+\mu^2\right)u'' - \alpha + u - u^2 v = 0 \\ -cv' - D_v\left(1+\mu^2\right)u'' - \beta + u^2 v = 0 \end{cases} \tag{7}$$

With the balancing principle, the ansatzes are determined as $u(\xi) = g_0 + g_1 z(\xi) + g_2 z^2(\xi)$ and $v(\xi) = h_0 + h_1\omega(\xi)$ where $g_i (i = 0, 1, 2)$ and $h_j (j = 0, 1)$ are parameters and will be determined as a result of the algebraic system, $z(\xi)$ and $\omega(\xi)$ are solutions of Bernoulli and Hermite differential equation, respectively. For the first equation of Eq. (7), Bernoulli type differential equation for $k = 2$ and Hermite differential equation for the second equation of Eq. (7) are considered as an auxiliary equation. Substituting the considered ansatzes and auxiliary equation in the system, the nonlinear algebraic equation system is obtained respect to the powers of $z(\xi)$ and $\omega(\xi)$. As a result, many solution sets are obtained that some of them gives trivial solutions, some of them are constant solutions. The useful solution sets are given in Table 1.

Therefore, substituting the obtained parameters into the ansatzes the analytical solutions are obtained that is the first attempt. Additionally, the considered methodology has not seen in the literature to our knowledge.

Table 1 The solution sets of the algebraic system

Set 1	$P = \frac{g_1 Q}{2g_2}, C_1 = 0, \alpha = 0, \beta = 0, c = -\frac{5g_2}{3Qg_1}, \lambda = 0, D_u = -\frac{g_2^2}{3Q^2 g_1^2}, g_0 = \frac{g_1^2}{4g_2}$
	$h_0 = -\frac{g_1^2 h_1 C_2 KummerU\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right)\xi - 4g_2}{g_1^2}$
Set 2	$Q = 0, \alpha = -\frac{g_2 + g_1 C_1 \exp(-P\xi)}{\exp(-P\xi)^2 C_1^2}, \beta = -\frac{h_1 C_1 \exp\left(\xi^2\right)(8D_v P\xi + 3)}{2P}, c = \frac{3}{2P}, \lambda = 0,$
	$D_u = -\frac{1}{4P^2}, g_0 = -\frac{g_2 + g_1 C_1 \exp(-P\xi)}{\exp(-P\xi)^2 C_1^2}, h_0 = -h_1\xi\left(C_1 KummerM\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right) + C_2 KummerU\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right)\right)$
Set 3	$Q = 2C_1 Pexp(-P\xi), C_2 = 0, \alpha = 0, c = \frac{5}{6P}, \lambda = 0, D_u = \frac{1}{12P^2}, g_0 = 0,$
	$D_v = -\frac{-6\beta P\xi g_2 KummerM\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right) + 5h_0 g_2 \exp\left(\xi^2\right) + 20C_1^2 \exp\left(\xi^2 - 2P\xi\right)}{24P\xi \exp\left(\xi^2\right)\left(g_2 h_0 + 4C_1^2 \exp(-P\xi)^2\right)}$
	$g_1 = \frac{g_2}{C_1 \exp(-P\xi)}, h_1 = -\frac{g_2 h_0 + 4C_1^2 \exp(-P\xi)^2}{g_2 C_1 \xi KummerM\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right)}$
Set 4	$Q = 2C_1 Pexp(-P\xi), C_2 = -\frac{h_0 g_2 + \xi g_2 h_1 C_1 KummerM\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right) + 4C_1^2 \exp(-P\xi)^2}{\xi g_2 h_1 KummerU\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right)}, \alpha = 0, c = \frac{5}{6P},$
	$\lambda = 0, D_u = \frac{1}{12P^2}, g_0 = 0, D_v = -\frac{6\beta P\xi + 5C_1 h_1 \xi \exp\left(\xi^2\right)}{24C_1 P\xi^2 h_1 \exp\left(\xi^2\right)}, g_1 = \frac{g_2}{C_1 \exp(-P\xi)}$

The Brusselator Model

The Brusselator model that is generally given as

$$\begin{cases} u_t = D_u \nabla^2 u + \alpha - (\beta + 1)u + f(u)v \\ v_t = D_v \nabla^2 v + \beta u - f(u)v \end{cases} \tag{8}$$

where D_u and D_v are the diffusion coefficients of the chemicals U and V, respectively. α and β are positive fixed concentration of the A and B, $f(u)$ is a nonnegative and nondecreasing function and assumed as $f(u) = u^2$ [1, 5].

Using the wave transformation $\xi = x + \mu y - ct$, $c \neq 0$, $\mu \neq 0$, the system is reduced into the following system;

$$\begin{cases} -cu' - D_u\left(1 + \mu^2\right)u'' - \alpha + (\beta + 1)u - u^2 v = 0 \\ -cv' - D_v\left(1 + \mu^2\right)u'' - \beta u + u^2 v = 0 \end{cases} \tag{9}$$

With the balancing principle, the ansatz is determined as $u(\xi) = g_0 + g_1\omega(\xi)$ and $v(\xi) = h_0 + h_1 z(\xi)$ where $g_i\,(i = 0, 1)$ and $h_j\,(j = 0, 1)$ are parameters and will be determined as a result of the algebraic system, $z(\xi)$ and $\omega(\xi)$ are solutions of Hermite and Bernoulli differential equation, respectively. For the first equation of Eq. (9), Hermite differential equation and Bernoulli type differential equation for $k = 2$ for the second equation of Eq. (9) are considered as an auxiliary equation. Substituting the considered ansatzes and auxiliary equation in the system, the nonlinear algebraic equation system is obtained respect to the powers of $z(\xi)$ and $\omega(\xi)$. As a result, many solution sets are obtained that some of them gives trivial solutions, some of them are constant solutions and lots of them have complex structure so not need to give here. Therefore, useful solution set is given as.

$$C_1 = 0, \alpha = 0, \beta = 0, \lambda = 0, D_v = -\frac{c}{2P}$$

$$g_0 = -g_1 C_2 \xi\, KummerU\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right), h_1 = \frac{Q\left(h_0 g_1 C_2 \xi\, KummerU\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right) + 1\right)\cdot}{P g_1 C_2 \xi\, KummerU\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right)}$$

The Lengyel–Epstein Model

The model is established on the time evolution of the concentrations of $\left[I^-\right]$ and $\left[ClO_2^-\right]$ which are represented by u and v, respectively [7],

$$\begin{cases} u_t = \nabla^2 u + \alpha - u - \dfrac{4uv}{1 + u^2} \\ v_t = d\nabla^2 v + \beta\left(u - \dfrac{uv}{1 + u^2}\right) \end{cases} \tag{10}$$

where α,$\beta > 0$ are rate constants that dependent on feed concentrations, d is the the diffusion coefficient.

Using the wave transformation $\xi = x + \mu y - ct$, $c \neq 0$, $\mu \neq 0$, the system is reduced into the following system;

$$\begin{cases} -c\left(1 + u^2\right)u' - \left(1 + \mu^2\right)\left(1 + u^2\right)u'' - \alpha\left(1 + u^2\right) + \left(1 + u^2\right)u - 4uv = 0 \\ -c\left(1 + u^2\right)v' - d\left(1 + \mu^2\right)\left(1 + u^2\right)u'' - \beta\left(1 + u^2\right)u + \beta uv = 0 \end{cases} \tag{11}$$

With the balancing principle, the ansatzes are determined as $u(\xi) = g_0 + g_1\omega(\xi)$ and $v(\xi) = h_0 + h_1 z(\xi)$ where $g_i\,(i = 0, 1)$ and $h_j\,(j = 0, 1)$ are parameters and will be determined as a result of the algebraic system, $z(\xi)$ and $\omega(\xi)$ are solutions of Hermite and Bernoulli

Table 2 The solution sets of the algebraic system

Set 1	$P=0,\alpha=-g_1C_1\exp\left(\xi^2\right)(c-4\xi),\beta=0,\lambda=0,h_0=\frac{1}{4},$ $g_0=I-g_1\xi\left(C_2KummerU\left(\frac{1}{2},\frac{3}{2},\xi^2\right)+C_1KummerM\left(\frac{1}{2},\frac{3}{2},\xi^2\right)\right)$
Set 2	$C_1=0,\alpha=0,\beta=0,c=-2dP,\lambda=0,h_1=\frac{Q(4h_0-1)}{4P}$
Set 3	$C_1=0,C_2=-\frac{g_0\left(g_0^2-3\right)}{g_1\left(g_0^2-1\right)\xi KummerU\left(\frac{2+\lambda}{4},\frac{3}{2},\xi^2\right)},\beta=0,c=-2dP,$ $\alpha=\frac{g_0\lambda}{4\xi\left(g_0^2-1\right)KummerU\left(\frac{2+\lambda}{4},\frac{3}{2},\xi^2\right)}\left(\begin{array}{l}KummerU\left(\frac{6+\lambda}{4},\frac{3}{2},\xi^2\right)\left(\begin{array}{l}-2dPg_0^2+6dP-dP\lambda g_0^2\\+3dP\lambda+4\xi g_0^2-12\xi+2\lambda\xi g_0^2-6\lambda\xi\end{array}\right)\\+KummerU\left(\frac{2+\lambda}{4},\frac{3}{2},\xi^2\right)\left(4dPg_0^2-12dP-16\xi g_0^2+16\xi\right)\end{array}\right)$ $h_1=-\frac{Q\left(2g_0^4\lambda+4\lambda g_0^2+g_0^2-1-4h_0g_0^2+4h_0+2\lambda\right)}{4\left(g_0^2-1\right)P}$
Set 4	$\alpha=-g_1C_1\exp\left(\xi^2\right)(c+4\xi),\beta=0,\lambda=0,g_0=I-g_1\xi\left(C_2KummerU\left(\frac{1}{2},\frac{3}{2},\xi^2\right)+C_1KummerM\left(\frac{1}{2},\frac{3}{2},\xi^2\right)\right)$ $h_1=-\frac{P-C_1P\exp(-P\xi)(1+4h_0)-4h_0P}{4P}$
Set 5	$C_1=0,\alpha=0,c=-2dP,\lambda=0,g_0=-g_1C_2KummerU\left(\frac{1}{2},\frac{3}{2},\xi^2\right)\xi,$ $h_0=1,h_1=\frac{3P}{4Q}$

Table 2 continued

Set 6	$P = 0, \alpha = -g_1 C_1 \exp\left(\xi^2\right)(c + 4\xi), \beta = 0, \lambda = 0, h_0 = \frac{1}{4},$
	$g_0 = I - g_1 \xi \left(C_2 KummerU\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right) + C_1 KummerM\left(\frac{1}{2}, \frac{3}{2}, \xi^2\right)\right)$
Set 7	$C_1 = 0, C_2 = -\frac{g_0\left(g_0^2 - 3\right)}{g_1\left(g_0^2 - 1\right)\xi KummerU\left(\frac{2+\lambda}{4}, \frac{3}{2}, \xi^2\right)}, \beta = 0, c = -2dP,$
	$\alpha = \frac{g_0 \lambda}{4\xi\left(g_0^2 - 1\right) KummerU\left(\frac{2+\lambda}{4}, \frac{3}{2}, \xi^2\right)} \left(\begin{array}{l} KummerU\left(\frac{6+\lambda}{4}, \frac{3}{2}, \xi^2\right)\left(\begin{array}{l} -2dPg_0^2 + 6dP - dP\lambda g_0^2 \\ +3dP\lambda + 4\xi g_0^2 - 12\xi + 2\lambda\xi g_0^2 - 6\lambda\xi \end{array}\right) \\ +KummerU\left(\frac{2+\lambda}{4}, \frac{3}{2}, \xi^2\right)\left(4dPg_0^2 - 12dP - 16\xi g_0^2 + 16\xi\right) \end{array}\right)$
	$h_1 = -\frac{Q\left(2g_0^6\lambda + 2\lambda g_0^4 - 2\lambda g_0^2 - 2\lambda - 3 - 10g_0^2 - 3g_0^4\right)}{(g_0 - 1)^2 (g_0 + 1)^2 P}, h_0 = \frac{g_0^4 + 2g_0^2 + 1}{\left(g_0^2 - 1\right)^2}$

differential equation, respectively. For the first equation of Eq. (11), Hermite differential equation and Bernoulli type differential equation for $k = 2$ for the second equation of Eq. (11) are considered as an auxiliary equation. Substituting the considered ansatzes and auxiliary equation in the system, the nonlinear algebraic equation system is obtained respect to the powers of $z(\xi)$ and $\omega(\xi)$. As a result, many solution sets are obtained that some of them gives trivial solutions, some of them are constant solutions and lots of them have complex structure so not need to give here. Therefore, the useful solution sets are given by Table 2.

Substituting the parameters into the ansatz, the exact solutions are obtained. The obtained results new in the literature to our knowledge and they have a major role in the literature so that the considered models are seen in a large scale of applications not only chemistry but also in biology.

Conclusion

Reaction–diffusion systems are used to model many physical, chemical, biological, environmental and even sociological processes [1]. In examining the chemical reaction–diffusion models, Schnakenberg, Brusselator and Lengyel–Epstein models are the most seen ones. These models are also known as Tuning-type models which have been used for generating patterns in both chemical and biological systems [1]. The exact solutions are not seen in the literature to our knowledge (all works in the literature are experimental and numerical solutions). The exact solutions of the considered models are obtained via the novel approach i.e. the combination of Bernoulli approximation method [15] and Hermite approximation method [17], each of the methods are seen as a modification of the well-known auxiliary equation method [13, 16]. The obtained results have a major role in the literature so that the considered models are seen in a large scale of applications not only chemistry but also in biology. For the future works, as seen in the literature, the fractional type of models can be considered.

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