

A Numerical Simulation and New Traveling Wave Solutions of Convection-Diffusion Equation with Reaction

E. E. El-Behadi

College of Science and Humanity Studies,
Mathematics Department, Salman bin
Abdulaziz, University, KSA.
h_feast@yahoo.com

M. A. Ashabrawy

*Community College, Computer Department,
Salman bin Abdulaziz University, KSA
*Reactors Department, Computer Group,
Atomic Energy Authority, Egypt
ashabrawy@hotmail.com

Abstract: Throughout this paper we will discuss and analyze of the convection-diffusion equation which included a reaction term. First, we will apply an alternating-direction implicit (ADI) scheme akin to that proposed by Pomezhaev. Use of this implicit operator-splitting scheme allows the application of a tridiagonal Thomas solver to obtain the solution of steady convection-diffusion equation with reaction. According to the unsteady case, we will use the improved (G'/G) -expansion method to construct the traveling wave solutions, where (G'/G) satisfies a second order linear ordinary differential equation. In this paper we will explore new applications of this method to some special nonlinear convection-diffusion equation with reaction.

Keywords: convection-diffusion-reaction equation, alternating-direction implicit (ADI) scheme, (G'/G) -expansion, traveling wave solutions, linear and nonlinear differential equations.

1. INTRODUCTION

In this paper, we will discuss and investigate two methods for solving a convection–diffusion–reaction (CDR) scalar transport equation. This equation is practically important because the working equations of many cases fall into this field. Typical examples are the Helmholtz equation for modeling exterior acoustics [1], constitutive equations for modeling the turbulent quantities k and ε [2], and viscoelastic constitutive equations for modeling the extra stresses in non-Newtonian fluid flows [3]. The main points in this research boils down to the following points. Section 2 presents the working equation, and then an alternating-direction implicit scheme, similar to that of Pomezhaev [4], is used to obtain the steady/transient CDR equation in one dimension. Throughout sections 3, 4, our emphasis in this paper is on the derivation of new traveling wave solutions of unsteady-state nonlinear CDR equation in one dimension [5, 6].

Since the most of phenomena in physics and other fields of mathematics are described by nonlinear evolution equations. And when we want to understand the physical meaning of phenomena, it was described by nonlinear evolution equations, and then exact solutions for the nonlinear evolution equations have to be explored. For example, the wave phenomena observed in fluid dynamics [7, 8], plasma and elastic media [9,10], etc. Recently, Wang et al [11, 12] introduced a new method called the the (G'/G) -expansion method to look for the traveling wave solutions of nonlinear evolution equations. Here we shall use a new improved (G'/G) -expansion method [13-19]. The main idea of this method is that the traveling wave solutions of nonlinear equations can be expressed by a polynomial in (G'/G) , where $G = G(\xi)$, where $\xi = x - \omega t$, satisfies the second order linear ODE $G'' + \lambda G' + \mu G = 0$, where λ, μ , and ω are constants. The degree of this polynomial can be determined by considering the homogeneous balance between the highest order derivatives and the nonlinear terms appearing in the given nonlinear equations [19-21]. The coefficients of this polynomial can be obtained by solving a set of algebraic equations resulting from the process of using the proposed method. In this paper, the

(G'/G) -expansion method will play an important role in expressing the traveling wave solutions of the convection-diffusion equation which included the reaction term.

2. WORKING EQUATIONS AND SOLUTION ALGORITHM

We consider firstly the scalar two dimensional convection–diffusion–reaction equation

$$\frac{\partial \phi}{\partial t} + V \cdot \nabla \phi - k \nabla^2 \phi + c \phi = 0 \tag{2.1}$$

Where $V = (u, v)$ represent the velocity components along the x and y directions, respectively. Other coefficients involve k and c , which denote the diffusion coefficient and the reaction coefficient, respectively. For illustrative purposes, all these values are assumed to be constant. For simplicity, the investigated equation is subject to the Dirichlet-type boundary condition $\phi = g$ on $\partial\Omega$, $t \in (0, T)$. Equation (2.1) with given boundary condition constitute a closure problem provided that the initial data of $\phi(x, y, 0)$ are prescribed. The strategy we will consider for solving (2.1) is similar to the ADI (alternating-direction implicit) scheme of Polezhaev.

By virtue of operator splitting, calculation of the approximated solution of Eq. (2.1) is accomplished in two steps, first is the *predictor step* and the second is the *corrector step*; respectively

$$\phi^* + \frac{\Delta t}{2} (u \phi_x^* - k \phi_{xx}^*) + \frac{\Delta t}{2} c \phi^* = \phi^n - \frac{\Delta t}{2} (v \phi_y^n - k \phi_{yy}^n) \tag{2.2a}$$

$$\phi^{n+1} + \frac{\Delta t}{2} (v \phi_y^{n+1} - k \phi_{yy}^{n+1}) + \frac{\Delta t}{2} c \phi^{n+1} = \phi^* - \frac{\Delta t}{2} (u \phi_x^* - k \phi_{xx}^*) \tag{2.2b}$$

Let us define

$$(u_1, v_1) = \left(\frac{\Delta t}{2} u, \frac{\Delta t}{2} v \right),$$

$$k_1 = \frac{\Delta t}{2} k \tag{2.3}$$

$$c_1 = 1 + \frac{\Delta t}{2} c$$

The above two-step ADI scheme for solving Eq. (2.1) can be rewritten as

$$u_1 \phi_x^* - k_1 \phi_{xx}^* + c_1 \phi^* = f_1 \tag{2.4a}$$

$$v_1 \phi_y^{n+1} - k_1 \phi_{yy}^{n+1} + c_1 \phi^{n+1} = f_2 \tag{2.4b}$$

Where the source terms f_1 and f_2 are given by

$$f_1 = \phi^n + v_1 \phi_y^n + k_1 \phi_{yy}^n \tag{2.5a}$$

$$f_2 = \phi^* - u_1 \phi_x^* + k_1 \phi_{xx}^* \tag{2.5b}$$

For the unsteady case, the scalar convection–diffusion–reaction equation in one dimension is of the form

$$\phi_t + u \phi_x - k \phi_{xx} + c \phi = 0 \tag{2.6}$$

We apply the semidiscretization scheme to approximate Eq. (2.6). In the time-stepping scheme, we consider $\phi_t = (\phi^{n+1} - \phi^n) / \Delta t$, which yields first-order accuracy. The resulting equation containing only the spatial derivatives is

$$\hat{u} \phi_x^{n+1} - \hat{k} \phi_{xx}^{n+1} + \hat{c} \phi^{n+1} = \phi^n \tag{2.7}$$

The definitions of \hat{u} , \hat{k} and \hat{c} are $\hat{u} = u \Delta t$, $\hat{k} = k \Delta t$, and $\hat{c} = 1 + c \Delta t$.

Equations (2.4a), (2.4b), and (2.7) are known as the steady-state convection–diffusion–reaction equations. At this point, we realize that the key to success in solving Eq. (2.1) lies in the analysis of the following model equation:

$$u\phi_x - k\phi_{xx} + c\phi = f \tag{2.8}$$

As is the case when a partial differential equation is simulated, we aim to obtain higher prediction accuracy. To this end, we employ the general solution for Eq. (2.8),

$$\phi = a e^{\lambda_1 x} + b e^{\lambda_2 x} + \frac{f}{c} \tag{2.9}$$

where a and b are constants. Substituting Eq. (2.9) into Eq. (2.8), we have two equations for λ_1 and λ_2 , respectively:

$$\begin{aligned} k\lambda_1^2 - u\lambda_1 - c &= 0, \\ k\lambda_2^2 - u\lambda_2 - c &= 0. \end{aligned} \tag{2.10}$$

The above two equations enable us to determine λ_1 and λ_2 as follows:

$$\lambda_{1,2} = \frac{u \pm \sqrt{u^2 + 4ck}}{2k}. \tag{2.11}$$

We will focus our attention now to the solution of the nonlinear type of equation (2.6) using the improved (G'/G) -expansion method [13-19].

3. DESCRIPTION OF THE (G'/G) -EXPANSION METHOD

Suppose that a nonlinear equation is given by

$$P(u, u_t, u_x, u_{tt}, u_{xt}, u_{xx}, \dots) = 0, \tag{3.1}$$

where $u = u(x, t)$ is an unknown function and P is a polynomial in $u = u(x, t)$ and its partial derivatives, in which the highest order derivatives and nonlinear terms are involved. In the following we give the main steps of the (G'/G) -expansion method.

Step 1: Combining the independent variables x and t into one variable $\xi = x - \omega t$, we suppose that

$$u(x, t) = u(\xi), \quad \xi = x - \omega t, \tag{3.2}$$

The travelling wave variable ξ permits us to reduce Eq. (3.1) to an ODE for $u = u(\xi)$, namely

$$P(u, -\omega u', u', \omega^2 u'', -\omega u'', u'', \dots) = 0 \tag{3.3}$$

Step 2: Suppose that the solution of ODE (3.3) can be expressed by a polynomial in (G'/G) as follows:

$$u(\xi) = \alpha_m \left(\frac{G'}{G}\right)^m + \dots, \tag{3.4}$$

where m is called the balance number and $G = G(\xi)$ satisfies the second order linear differential equation in the form

$$G'' + \lambda G' + \mu G = 0, \tag{3.5}$$

where $\alpha_m, \alpha_{m-1}, \dots, \alpha_0, \lambda, \mu$ are constants to be determined later, $\alpha_m \neq 0$. Using the general solution of Eq. (3.5), we have

$$\left(\frac{G'}{G}\right) = \begin{cases} \frac{\sqrt{\lambda^2 - 4\mu}}{2} \left(\frac{c_1 \sinh\left(\frac{\sqrt{\lambda^2 - 4\mu}}{2} \xi\right) + c_2 \cosh\left(\frac{\sqrt{\lambda^2 - 4\mu}}{2} \xi\right)}{c_1 \cosh\left(\frac{\sqrt{\lambda^2 - 4\mu}}{2} \xi\right) + c_2 \sinh\left(\frac{\sqrt{\lambda^2 - 4\mu}}{2} \xi\right)} \right) - \frac{\lambda}{2}, & \lambda^2 - 4\mu > 0, \\ \frac{\sqrt{4\mu - \lambda^2}}{2} \left(\frac{-c_1 \sin\left(\frac{\sqrt{4\mu - \lambda^2}}{2} \xi\right) + c_2 \cos\left(\frac{\sqrt{4\mu - \lambda^2}}{2} \xi\right)}{c_1 \cos\left(\frac{\sqrt{4\mu - \lambda^2}}{2} \xi\right) + c_2 \sin\left(\frac{\sqrt{4\mu - \lambda^2}}{2} \xi\right)} \right) - \frac{\lambda}{2}, & \lambda^2 - 4\mu < 0. \end{cases} \quad (3.6)$$

The unwritten part in Eq. (3.4) is also a polynomial in (G'/G) , but the degree of which is equal or less than $m-1$. The positive integer m can be determined by considering the homogeneous balance between the highest order derivatives and nonlinear terms appearing in ODE (3.3).

Step 3: By substituting (3.4) into (3.3) and using (3.5), collecting all terms with the same order of (G'/G) together, and then equating each coefficient of the resulting polynomial to zero yields a set of algebraic equations for $\alpha_m, \alpha_{m-1}, \dots, \alpha_0, \omega, \lambda$ and μ .

Step 4: Assuming that the constants $\alpha_m, \alpha_{m-1}, \dots, \alpha_0, \omega, \lambda$ and μ can be obtained by solving the algebraic equations in Step 3, since the general solutions of the second order linear ODE (3.5) is well known for us, then substituting $\alpha_m, \alpha_{m-1}, \dots, \alpha_0, \omega$, and the general solutions of Eq. (3.5) into (3.4) we have more travelling wave solutions of the nonlinear evolution Eq. (3.1).

In the subsequent sections, we will illustrate the validity and reliability of this method in detail with some nonlinear evolution equations in mathematical physics the balance numbers of which are not positive integers.

4. APPLICATION TO THE CDR EQUATION

In this section, we will apply the (G'/G) -expansion method to construct the traveling solutions for CDR [5,6]

$$\phi_t + u\phi_x - k\phi_{xx} + F = 0 \quad (4.1)$$

Where the reaction term F is a source. We remark that geologists, civil engineers, mathematicians, and so on, frequently use different terminology in describing the phenomena embodied in equation (4.1). As found in [5], if the tracer is radioactive with decay rate c , then $F = c\phi$ and we obtain the linear CDR Eq. (2.6).

If the tracer is a biological species with *logistic growth* rate $F = r\phi(1 - \frac{\phi^p}{R})$, where r is the growth constant, R is the carrying capacity, and $p(\neq 1)$ is a positive quantity. Then we start with the CDR equation (convection-diffusion equation with growth) in the form

$$\phi_t + u\phi_x - k\phi_{xx} + \alpha\phi - \beta\phi^p = 0 \quad (4.2)$$

Where k, α and β are nonzero constants. The traveling wave variable below,

$$\phi(x, t) = \phi(\xi), \quad \xi = x - \omega t \quad (4.3)$$

Permits us to convert Eq. (4.2) into an ODE for $\phi(x, t) = \phi(\xi)$ in the form

$$\alpha\phi + (u - \omega)\phi' - k\phi'' - \beta\phi^p = 0, \quad (4.4)$$

where ω is a constant. Suppose that the solution of the ODE (4.4) can be expressed by a polynomial in (G'/G) as follows:

$$\phi(\xi) = \alpha_m \left(\frac{G'}{G}\right)^m + \dots, \quad (4.5)$$

where $G = G(\xi)$ satisfies Eq. (3.5).

By using (4.5) and (3.5), it is easily derived that

$$\phi^p(\xi) = \alpha_m^p \left(\frac{G'}{G}\right)^p + \dots, \tag{4.6}$$

$$\phi''(\xi) = m(m+1)\alpha_m \left(\frac{G'}{G}\right)^{m+2} + \dots \tag{4.7}$$

Considering the homogeneous balance between ϕ^p and ϕ'' in (4.4), based on (4.6) and (4.7), we required that $pm = m + 2 \Rightarrow m = \frac{2}{p-1}$. It should be noticed that m is not a positive integer. However, we may choose the solution of Eq. (4.4) in the form

$$\phi(\xi) = A \left(\frac{G'}{G}\right)^{\frac{2}{p-1}}, \tag{4.8}$$

where A is a real constant to be determined later and G satisfies Eq. (3.5). It is easy to deduce that

$$\phi' = -\frac{2}{p-1} A \left(\frac{G'}{G}\right)^{\frac{p+1}{p-1}} - \frac{2}{p-1} A \lambda \left(\frac{G'}{G}\right)^{\frac{2}{p-1}} - \frac{2}{p-1} A \mu \left(\frac{G'}{G}\right)^{\frac{-p+3}{p-1}} \tag{4.9}$$

$$\begin{aligned} \phi'' = & \frac{2(p+1)}{(p-1)^2} A \left(\frac{G'}{G}\right)^{\frac{2p}{p-1}} + \frac{2(p+3)}{(p-1)^2} A \lambda \left(\frac{G'}{G}\right)^{\frac{p+1}{p-1}} + \frac{4}{(p-1)^2} A (2\mu + \lambda^2) \left(\frac{G'}{G}\right)^{\frac{2}{p-1}} \\ & + \frac{2(-p+5)}{(p-1)^2} A \lambda \mu \left(\frac{G'}{G}\right)^{\frac{-p+3}{p-1}} + \frac{2(-p+3)}{(p-1)^2} A \mu^2 \left(\frac{G'}{G}\right)^{\frac{2(-p+2)}{p-1}} \end{aligned} \tag{4.10}$$

Substituting (4.8) – (4.10) into (4.4) and collecting all terms with the same powers of (G'/G) together, we obtain

$$-\frac{2(p+1)}{(p-1)^2} Ak - A^p \beta = 0, \tag{4.11}$$

$$-\frac{2}{(p-1)} A(u - \omega) - \frac{2(p+3)}{(p-1)^2} A \lambda k = 0, \tag{4.12}$$

$$\alpha A - \frac{2}{(p-1)} A \lambda (u - \omega) - \frac{4}{(p-1)^2} A (2\mu + \lambda^2) k = 0, \tag{4.13}$$

$$-\frac{2}{(p-1)} A \mu (u - \omega) - \frac{2(-p+5)}{(p-1)^2} A \lambda \mu k = 0, \tag{4.14}$$

$$-\frac{2(-p+3)}{(p-1)^2} A \mu^2 k = 0. \tag{4.15}$$

Solving the above algebraic equations (4.11)-(4.15), we have

$$A = 2^{\frac{1}{p-1}} \left(\frac{-\beta(p-1)^2}{k(p+1)} \right)^{\frac{-1}{p-1}} \tag{4.16}$$

$$\lambda = \pm \sqrt{\frac{-\alpha}{2k}} \frac{p-1}{\sqrt{p+1}} \tag{4.16}$$

$$\omega = u \pm \lambda \left(k + \frac{4k}{p-1} \right)$$

$$\mu = 0$$

Substituting (4.16) into (3.7) yields

$$\phi(\xi) = 2^{\frac{1}{p-1}} \left(\frac{-\beta(p-1)^2}{k(p+1)} \right)^{\frac{-1}{p-1}} \left(\frac{G'}{G} \right)^{\frac{2}{p-1}} \tag{4.17}$$

where

$$\xi = x - \left(u \pm \lambda \left(k + \frac{4k}{p-1} \right) \right) t. \tag{4.18}$$

Using Eq. (3.6) we deduce after some reduction that

$$\left(\frac{G'}{G} \right) = \lambda \left(\frac{c_2 e^{-\lambda \xi}}{c_1 - c_2 e^{-\lambda \xi}} \right) \tag{4.19}$$

Where c_1 and c_2 are arbitrary constants. Substituting (4.19) into (4.17), we obtain the new exact traveling wave solution of Eq. (4.2) as follows:

$$\phi(x, t) = 2^{\frac{1}{p-1}} \left(\frac{-\beta(p-1)^2}{k(p+1)} \right)^{\frac{-1}{p-1}} \lambda \left(\frac{c_2 e^{-\lambda \xi}}{c_1 - c_2 e^{-\lambda \xi}} \right)^{\frac{2}{p-1}}, \tag{4.20}$$

where λ and ξ are given above. If we chose $c_1 = c_2$ in (4.20), then we obtain the envelope solitary wave solutions of Eq. (4.20)

$$\phi(x, t) = 2^{\frac{-1}{p-1}} \left(\frac{(p-1)\beta}{k} \right)^{\frac{1}{p-1}} \lambda \left(\frac{1}{2} - \frac{1}{2} \tanh\left(\frac{-\lambda \xi}{2}\right) \right)^{\frac{2}{p-1}} \tag{4.21}$$

As a special Case: if we put $p=2$ in Eq. (4.2), then we have

$$A = \frac{-6k}{\beta}, \quad \lambda = \pm \sqrt{\frac{-\alpha}{6k}}, \quad \omega = u \pm 5k\lambda, \quad \mu = 0. \tag{4.22}$$

And therefore its solution, in this case, takes the form

$$\phi(\xi) = \frac{-6\beta}{k} \lambda \left(\frac{c_2 e^{-\lambda \xi}}{c_1 - c_2 e^{-\lambda \xi}} \right)^2, \tag{4.23}$$

Where

$$\xi = x - (u \pm 5k\lambda) t. \tag{4.24}$$

Note that Eq. (4.23) represents the solitary wave solution of the convection-diffusion-reaction equation (4.2) in the case when $p=2$.

5. CONCLUSIONS

Throughout this research we have presented an alternating-direction implicit scheme, which is similar to Polezhave's scheme, to reduce 2D convection-diffusion-reaction equation into steady-state one-dimensional one. The main discussion here is to find a new solution of unsteady-state CDR using (G'/G) -expansion method. Since the (G'/G) -expansion method was presented by Wang, this method has been improved by several authors. However, the application of this method was still limited to those equations the balance numbers of which are positive integers. In this paper, we explore a new application of the (G'/G) -expansion method and obtain new types of exact travelling wave solutions to a kind of nonlinear CDR equation. This paper presents a wider applicability for handling nonlinear evolution equations using the (G'/G) -expansion method. The new type of exact travelling wave solution obtained in this paper might have significant impact on future researches. It is worthy of further study.

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AUTHORS' BIOGRAPHY



Dr. Eid Alsaid Eid Elbehadi obtained B.Sc. mathematics in 1989, M.Sc. applied mathematics in 1996 and Ph.D applied mathematics, fluid Mechanics especially computational fluid mechanics in 2003 from the Department of mathematics, Zagazig University, Egypt.



Dr. Mohamed Abdel Fatah Ashabrawy obtained B.Sc. Computer Science in 1996, M.Sc. Computer Science in 2002 and Ph.D Computer Science, Image processing, Medical image processing in 2010 from the Department of Computer Science, Suez canal University, Assistant Professor in Reactors Department, Nuclear Research Center , Atomic Energy Authority Egypt.