

Traveling-wave solution of non-linear coupled reaction diffusion equation arising in mathematical chemistry

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Received: 15 June 2008 / Accepted: 6 October 2008 / Published online: 28 October 2008
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Abstract A simple analytical approach to find the traveling-wave solution for a set of two coupled non-linear reaction diffusion equations is reported. An exact analytical solution for traveling-waves of the Fisher equations with a general non-linearity is found. The boundary value, the boundedness and the stability of the solution are discussed. This technique is straight forward to use involving minimal algebra. Use of the method for selected case is demonstrated.

Keywords Traveling-wave solutions · Non-linear reaction diffusion equations · Fisher equations

1 Introduction

Non-linear phenomena play a very important role in physics [1], chemistry and biology (heat and mass transfer, filtration of liquids, diffusion in chemical reactions, etc.). In particular in physics, non-linear waves are encountered in numerous domains such as fluid mechanics [2], solid-state physics [3], plasma physics [4] and chemical physics [5]. New names like solitons, kinks, breathers, etc. are now commonly used in the vast literature [6] dealing with this subject. Unfortunately these topics are treated only in advanced courses and can rarely be found on an introductory level. Therefore, simple techniques and methods are needed to investigate these phenomena and to make them accessible for undergraduate study.

Construction of particular exact solutions for the non linear equations remains an important problem. Finding exact solutions that have a physical, chemical or biological interpretation is of fundamental importance. Linear superposition principle cannot

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be applied to find the solution non-linear differential equations. Thus, the standard methods are not applicable for solving non-linear partial differential equations. A key step in investigating these problems is the derivation of traveling-waves from the associated (one-dimensional) wave equations. However, in contrast with linear wave theory where one can make use of the basic techniques, a variety of methods (inverse scattering method and the Lie method, etc.) and often involving complex mathematical technique is used for the solution of non-linear problems. The aim of this paper is to propose a unifying method that leads to straight forward solutions.

2 Mathematical formulation of the problem

We consider a set of one-dimensional non-linear reaction diffusion equation with diffusion described by Fick's law leads to the following equations [7]

$$\frac{\partial S}{\partial T} = D_S \frac{\partial^2 S}{\partial X^2} - \frac{V_{\max} S}{K_M + S} \quad 0 < X < 1, \quad 0 < T \leq \tau \quad (1)$$

$$\frac{\partial P}{\partial T} = D_P \frac{\partial^2 P}{\partial X^2} + \frac{V_{\max} S}{K_M + S} \quad 0 < X < 1, \quad 0 < T \leq \tau \quad (2)$$

Using the following parameters,

$$s = \frac{S}{\kappa S^\infty}, p = \frac{P}{\kappa S^\infty}, x = \frac{X}{L}, t = \frac{D_s T}{L^2}, \alpha = \frac{\kappa S^\infty}{K_M}, K = \frac{V_{\max} L^2}{K_M D_s}$$

we obtained the following dimensionless non-linear reaction diffusion equations

$$\frac{\partial s}{\partial t} = \frac{\partial^2 s}{\partial x^2} - \frac{K s}{1 + \alpha s} \quad 0 < t < 1, \quad 0 < t \leq \tau \quad (3)$$

$$\frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial x^2} + \frac{K s}{1 + \alpha s} \quad 0 < t < 1, \quad 0 < t \leq \tau \quad (4)$$

where s and p represents the dimensionless concentration of substrate and product while x and t represents dimensionless distance and time parameter, respectively. The parameter α denotes the saturation of the enzyme and K denotes reaction diffusion parameter. When $\alpha s < 1$, Eqs. 3 and 4 becomes

$$\frac{\partial s}{\partial t} = \frac{\partial^2 s}{\partial x^2} - K s (1 - \alpha s) \quad (5)$$

$$\frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial x^2} + K s (1 - \alpha s) \quad (6)$$

Since $s = 1 - p$, it is enough to solve Eq. 5 only. This type of non-linear diffusion equation is come across in chemical kinetics [5], population dynamics [1] and non-linear waves [8]. Such non-linear equations also occur often in the description of

chemical [9] and biological phenomena [10–13]. Using tanh method, we obtain (see Appendix 1 steps 1–3)

$$cv(1 - Y^2) \frac{dU(Y)}{dY} + c^2(1 - Y^2) \left(-2Y \frac{dU(Y)}{dY} + (1 - Y^2) \frac{d^2U(Y)}{dY^2} \right) - KU(Y) + \alpha K [U(Y)]^2 = 0 \quad (7)$$

Balancing the order of the non-linear term $[U(Y)]^2$ with the order of the Y^3 (or Y^4) component of the second term gives:

$$2M = 3 + M - 1 \text{ (or } 4 + M - 2\text{) such that } M = 2. \quad (8)$$

Hence,

$$U(Y) = a_0 + a_1 Y + a_2 Y^2 \quad (9)$$

Equating the coefficients of same power of Y^m ($m = 0, 1, 2, 3$ and 4), we get:

$$Y^0 \text{coeff.: } a_1 cv + 2a_2 c^2 - Ka_0 + \alpha K a_0^2 = 0, \quad (10)$$

$$Y^1 \text{coeff.: } 2a_2 cv - 2a_1 c^2 - Ka_1 + 2\alpha K a_0 a_1 = 0, \quad (11)$$

$$Y^2 \text{coeff.: } -a_1 cv - 8a_2 c^2 - Ka_2 + \alpha K a_1^2 + 2\alpha K a_1 a_2 = 0, \quad (12)$$

$$Y^3 \text{coeff.: } -2a_2 cv + 2a_1 c^2 + 2\alpha K a_1 a_2 = 0 \quad (13)$$

$$Y^4 \text{coeff.: } 6a_2 c^2 - \alpha K a_2^2 = 0, \quad (14)$$

Solving the above equations, we obtain the values of the following unknowns.

$$c^2 = K/24, v = 10c, a_0 = (K + 12c^2)/2\alpha K, a_1 = 6cv/5\alpha K, a_2 = -6c^2/\alpha K \quad (15)$$

(or)

$$a_0 = 3/4\alpha, a_1 = 1/2\alpha, a_2 = -1/4\alpha, v = 5\sqrt{K/6}, c = \frac{\sqrt{K/6}}{2} \quad (16)$$

Therefore

$$s(x, t) = \frac{1}{\alpha} - \frac{1}{4\alpha} \{1 - \tanh[c(x - vt)]\}^2 \quad (17)$$

Substituting the values of the constants c and v in eqn. (17), we obtain

$$s(x, t) = \frac{1}{\alpha} - \frac{1}{4\alpha} \left\{ 1 - \tanh \left[\frac{\sqrt{K/6}}{2} (x - 5\sqrt{K/6}t) \right] \right\}^2 \quad (18)$$

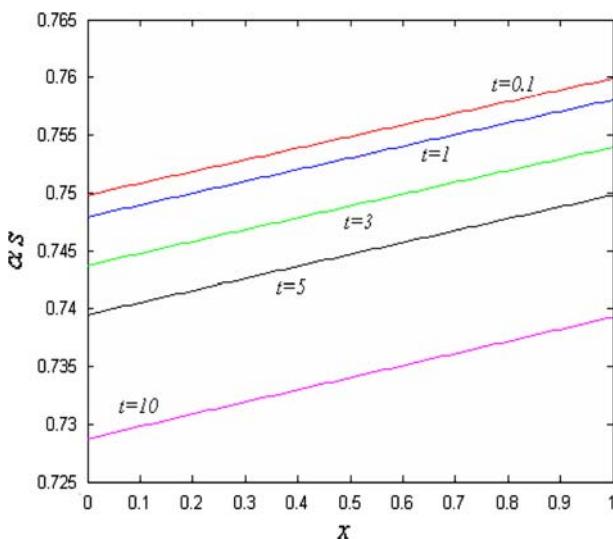


Fig. 1 Concentration $\alpha s(x, t)$ calculated using Eq. 18 for various values of t when $K = 0.01$

This is the exact solution of Fisher equation (5). Using the relation $s = 1 - p$, we can also obtain the solution of Eq. 6. Tables 1–3 indicate the values of substrate concentrations for various values of α , t and K . From the tables, it is inferred that the values of $s(x, t)$ decreases for all values of α and K when t increases. The values of $s(x, t)$ are constant, when $\alpha > 0.5$ for all values of x . The values of $s(x, t)$ become zero when $t \geq 3$, $K \geq 10$ for all values of α . Figures 1–3 shows the traveling-wave solution of substrate concentration $\alpha s(x, t)$ at $K = 0.01, 1, 5$, respectively. When t decreases the values of $\alpha s(x, t)$ increases for all values of K . The values of $\alpha s(x, t)$ become zero when $K \geq 1$ and $t \geq 5$. The function $\alpha s(x, t)$ is linear when t is constant. It is also more convenient to recast the Eq. 18 using the relation $1 - \tanh y = 2/[1 + e^{2y}]$ into the following format

$$s(z) = \frac{1}{\alpha} \left\{ 1 - \left[1 / \left[1 + \exp \left(z \sqrt{K/6} \right) \right]^2 \right] \right\} \quad (19)$$

where

$$z = x - 5\sqrt{K/6t} \quad (20)$$

Equation 19 is also derived in Appendix 1 using Murray [14] method. Figure 4 shows the traveling-wave solution of substrate concentration $\alpha s(z)$ at $K = 0.1, 1, 10$, respectively. The values of $\alpha s(z)$ increases when K increases.

Table 1 The numerical values of subtract $s(x, t)$ for various values of K and t when $\alpha = 0.01$

x	$s(x, t)$	$K = 0.01, \alpha = 0.01$						$K = 1, \alpha = 0.01$						$K = 10, \alpha = 0.01$					
		$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 7$	$t = 10$	$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 7$	$t = 10$	$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 7$	$t = 10$
0.00	74.9792	51.4108	14.5962	3.0301	0.5831	0.0481	72.8745	51.4108	14.5962	3.0301	0.5831	0.0481	51.4108	0.0481	0.0000	0.0000	0.0000	0.0000	
0.25	75.2338	54.4261	15.9716	3.3475	0.6454	0.0532	75.4660	54.4261	15.9716	3.3475	0.6454	0.0532	60.9446	0.0664	0.0000	0.0000	0.0000	0.0000	
0.5	75.4871	57.4491	17.4564	3.6972	0.7144	0.0589	77.9251	57.4491	17.4564	3.6972	0.7144	0.0589	70.0986	0.0916	0.0000	0.0000	0.0000	0.0000	
0.75	75.7390	60.4589	19.0553	4.0822	0.7907	0.0653	80.2405	60.4589	19.0553	4.0822	0.7907	0.0653	78.2543	0.1265	0.0000	0.0000	0.0000	0.0000	
1.00	75.9897	63.4339	20.7724	4.5059	0.8752	0.0723	82.4038	63.4339	20.7724	4.5059	0.8752	0.0723	84.9812	0.1746	0.0000	0.0000	0.0000	0.0000	

Table 2 The numerical values of subtract $s(x, t)$ for various values of K and t when $\alpha = 0.5$

x	$s(x, t)$	$K = 0.01, \alpha = 0.05$						$K = 1, \alpha = 0.05$						$K = 10, \alpha = 0.05$					
		$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 7$	$t = 10$	$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 7$	$t = 10$	$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 7$	$t = 10$
0.00	1.4996	1.4958	1.4874	1.4790	1.4704	1.4575	1.4575	1.0282	0.2919	0.0606	0.0117	0.0010	0.0282	0.0010	0.0000	0.0000	0.0000	0.0000	
0.25	1.5047	1.5009	1.4926	1.4841	1.4757	1.4628	1.5093	1.0885	0.3194	0.0669	0.0129	0.0011	1.2189	0.0013	0.0000	0.0000	0.0000	0.0000	
0.5	1.5097	1.5060	1.4977	1.4893	1.4809	1.4681	1.5585	1.1490	0.3491	0.0739	0.0143	0.0012	1.4020	0.0018	0.0000	0.0000	0.0000	0.0000	
0.75	1.5148	1.5111	1.5028	1.4945	1.4860	1.4733	1.6048	1.2092	0.3811	0.0816	0.0158	0.0013	1.5651	0.0025	0.0000	0.0000	0.0000	0.0000	
1.00	1.5198	1.5161	1.5079	1.4996	1.4912	1.4785	1.6481	1.2687	0.4154	0.0901	0.0175	0.0014	1.6996	0.0035	0.0000	0.0000	0.0000	0.0000	

Table 3 The numerical values of subtract $s(x, t)$ for various values of K and t when $\alpha = 1$

x	$s(x, t)$						$K = 0.01, \alpha = 1$						$K = 10, \alpha = 1$					
	$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 7$	$t = 10$	$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 7$	$t = 10$	$t = 0.1$	$t = 1$	$t = 3$	$t = 5$	$t = 7$	$t = 10$
0.00	0.7498	0.7479	0.7437	0.7395	0.7352	0.7287	0.7287	0.5141	0.1460	0.0303	0.0058	0.0005	0.5141	0.0005	0.0005	0.0005	0.0005	0.0000
0.25	0.7523	0.7505	0.7463	0.7421	0.7378	0.7314	0.7547	0.5443	0.1597	0.0335	0.0065	0.0005	0.6094	0.0007	0.0007	0.0007	0.0007	0.0000
0.5	0.7549	0.7530	0.7489	0.7447	0.7404	0.7340	0.7793	0.5745	0.1746	0.0370	0.0071	0.0006	0.7010	0.0009	0.0009	0.0009	0.0009	0.0000
0.75	0.7574	0.7555	0.7514	0.7472	0.7430	0.7367	0.8024	0.6046	0.1906	0.0408	0.0079	0.0007	0.7825	0.0013	0.0013	0.0013	0.0013	0.0000
1.00	0.7599	0.7581	0.7539	0.7498	0.7456	0.7393	0.8240	0.6343	0.2077	0.0451	0.0088	0.0007	0.8498	0.0017	0.0017	0.0017	0.0017	0.0000

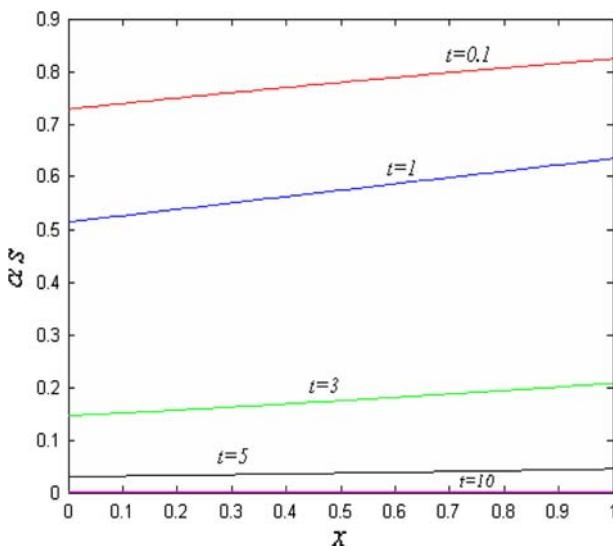


Fig. 2 Concentration $\alpha_s(x, t)$ calculated using Eq. 18 for various values of t when $K = 1$

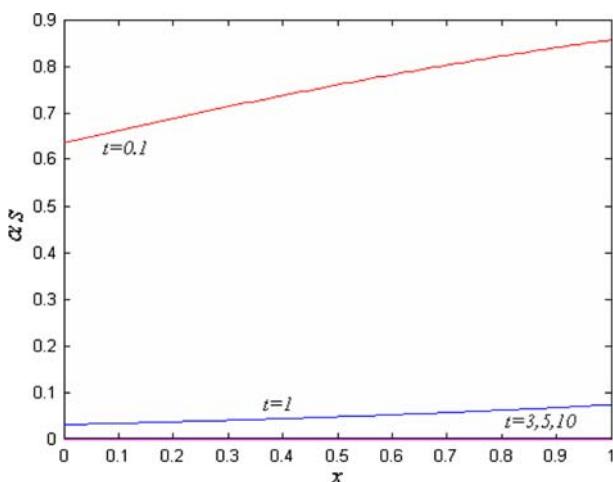


Fig. 3 Concentration $\alpha_s(x, t)$ calculated using Eq. 18 for various values of t when $K = 5$

3 Conclusion

We have presented a formal closed form of traveling-wave solutions of two coupled non-linear reaction diffusion equations. This procedure is straight forward to use and only nominal algebra is required. This method can be easily extended to find the solution of all other non-linear reaction diffusion equations.

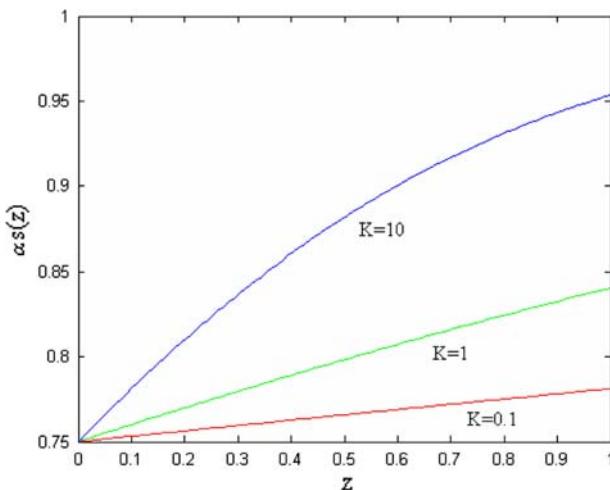


Fig. 4 Concentration $\alpha s(z)$ calculated using Eq. 19 for various values of K

Appendix 1

The starting point is a non-linear partial differential equation, which describes the dynamical evolution of the wave form $s(x, t)$. The following steps are then applied.

Step 1: A traveling-wave solution requires one coordinate:

$$\xi = c(x - vt) \text{ and thus } s(x, t) = U(\xi), \quad (21)$$

where $U(\xi)$ represents the (localized) wave solution, which travels with speed v . It exemplifies a stationary wave with a characteristic width $L = c^{-1}$. Without loss of generality we define $c > 0$. As a consequence, the derivatives are changed into

$$\frac{\partial}{\partial t} \rightarrow -cv \frac{d}{d\xi} \quad (22)$$

$$\frac{\partial}{\partial x} \rightarrow c \frac{d}{d\xi} \quad (23)$$

Step 2: After performing Step 1, we see that the partial differential equation becomes an ordinary differential equation.

Step 3: The ordinary differential equation is integrated as long as all terms contain derivatives. This procedure comes to an end when one of the terms contains no derivatives. The associated integration constants are taken to be zero, in view of the localized solutions we are looking for.

Step 4: The crucial step now is the introduction of $Y = \tanh(\xi)$ as a new independent variable. The corresponding derivatives are then changed as follows:

$$\frac{d}{d\xi} \rightarrow (1 - Y^2) \frac{d}{dY} \quad (24)$$

$$\frac{d^2}{d\xi^2} \rightarrow (1 - Y^2) \left(-2Y \frac{d}{dY} + (1 - Y^2) \frac{d^2}{dY^2} \right) \quad (25)$$

$$\begin{aligned} \frac{d^3}{d\xi^3} \rightarrow & -2Y(1 - Y^2) \left(-2Y \frac{d}{dY} + (1 - Y^2) \frac{d^2}{dY^2} \right) \\ & +(1 - Y^2)^2 \left(-2 \frac{d}{dY} - 2Y \frac{d^2}{dY^2} + (1 - Y^2) \frac{d^3}{dY^3} \right) \end{aligned} \quad (26)$$

Step 5: The solution may be expressed in terms of Y . There is no general procedure at this final stage. Often, the following series expansion is most favourable:

$$Z(Y) = \sum_{m=0}^M a_m Y^m \quad (27)$$

The parameter M can be found by balancing the linear terms(s). The linear term of highest order is contained in the highest derivative when applied to $S(Y)$. This is readily seen using the set of relations (24)–(26). The Y^2 component of Eq. 24 leads to the order $(2 + M - 1) = M + 1$, the Y^3 component of the first and the Y^4 component of the second derivative of Eq. 25 both lead to the order $M + 2$, etc. On the other hand, the non-linear terms yield multiples of M . The highest-order contribution of the latter must be equal to the former result. In this way the value of M is determined. Normally M will be a positive integer so that a closed analytical solution can be obtained. However, we have found one example where M takes a negative value. To avoid singularities for $Y \rightarrow 0$ in that case $-1 \leq Y \leq 1$, the series expansion (27) must be changed. As an obvious choice, we introduce

$$\left(\sum_{m=0}^M a_m Y^m \right)^{-1} \text{ with } M' = -M (> 0) \quad (28)$$

In principle, an infinite value for M is also allowed. It can be used in those cases where a finite value of M does not lead to a solution. But such cases are not treated here. Finally, the series expansion (27) and (28) is substituted into the relevant equation and recursion relations appear because the coefficients of Y^m ($m = 0, 1, 2, \dots, M$) have to vanish. From these relations, the coefficients a_m ($m = 0, 1, 2, \dots, M$) are then calculated.

Appendix 2

Derivation of solution of Fisher equation in exponential form

It is more convenient to recast Eq. 5 into the following format

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + Ku(1-u) \quad (29)$$

where

$$1 - \alpha s = u \quad (30)$$

Substituting $z = x - ct$ and $u(x, t) = U(z)$ in Eq. 29, we obtain the following ordinary differential equation.

$$L(U) = U'' + cU' + KU(1 - U) = 0 \quad (31)$$

We seek the solution of the above equation in the form [14]

$$U(z) = \left[1 + ae^{bz} \right]^{-2} \quad (32)$$

where a , b and c are positive constants, to be found. The arbitrary constants a cannot depend on b and c [14]. Substitution of Eq. 32 in Eq. 31 gives

$$6a^2b^2e^{2bz}(1+ae^{bz})^{-4} - 2ab^2e^{bz}(1+ae^{bz})^{-3} \\ - 2abce^{bz}(1+ae^{bz})^{-3} + K[1+ae^{bz}]^{-2}[1 - (1+ae^{bz})^{-2}] = 0 \quad (33)$$

The coefficients of e^{bz} and e^{2bz} are

$$K = b(b+c) \quad (34)$$

$$4b^2 - 2bc + K = 0 \quad (35)$$

Solving the above equations, we obtain the following relations

$$b = \sqrt{K/6}, \quad c = 5\sqrt{K/6} \quad (36)$$

The exact solution of Fisher Eq. 29 becomes

$$u(x, t) = U(z) = \left[1 + ae^{z\sqrt{K/6}} \right]^{-2} \quad (37)$$

where

$$z = x - 5t\sqrt{K/6} \quad (38)$$

When $K = 1$, the Eq. 37 is identical to equation (13.47) of Ref. [14]. The arbitrary constant a is depend upon the boundary condition $U(z=0)$. By choosing the constant $a = 1$ in Eq. 37 and using the relation (30), we obtain Eq. 19 in the text.

Acknowledgements The authors are very thankful to the referees for their valuable suggestion. The author also thanks to T. V. Krishnamurthy, The Principal and M. S. Meenakshisundaram, the Secretary of Madura College, Madurai, and the Vice Chancellor of Alagappa University, Karaikudi, for their encouragement. The author thanks to Prof. N. Thigarajan, Head of Department of Mathematics, The Madura College, Madurai, and Prof. N. Palaniappan, Department of Mathematics, Alagappa University, Karaikudi for useful discussion.

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