REACTION-DIFFUSION EQUATIONS: A CHEMICAL APPLICATION

RESUMEN

Obtenemos soluciones exactas para un sistema de reacción-difusión asociado a una reacción cubica autocatalítica entre dos sustancias químicas según la regla $A + B \rightarrow 2B$ con tasa $r = \rho ab$. Para obtener dichas soluciones empleamos una transformación de onda.

PALABRAS CLAVES: Ecuación RD, ecuaciones de reacción-difusión, solución de onda viajera, reacción autocatalítica.

ABSTRACT

We give exact solutions to a reactions-diffusion system corresponding to cubic autocatalytic reaction between two chemicals according to the rule $A + B \rightarrow 2B$ with rate $r = \rho ab$. We apply a traveling wave transformation in order to obtain these solutions.

KEYWORDS: *RD equation, reaction-diffusion equations, traveling wave solution, autocatalytic reaction.*

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1. Introduction

A question (Scott, 2005, pp. 783) is: How did life appear and develop on Earth? Although there is not complete agreement, a convincing answer is that given the required conditions (which were almost surely satisfied billions of years ago), life spontaneously emerged through the endless battle of survival of the fittest from a primordial chemical soup. The theory of random catalytic networks (Kauffman, 1995) shows that autocatalytic reactions are likely in this context; thus, the theory of interactions between chemical reactions and molecular diffusion takes center stage in emergence of biological life from atoms and molecules in a system.

Today, reaction-diffusion systems have found many applications ranging from chemical and biological phenomena to medicine (physiology, diseases, etc.), genetics, physics, social science, finance, economics, weather prediction, astrophysics, and so on (Aronson & Weinberger, 1975; Grindrod, 1996; Murray, 2002; Scott,

2003). Even for phenomena that bear no initial resemblance to these processes, it is sometimes useful and productive to use the reaction-diffusion metaphor in order to gain insight into their dynamics.

An important contribution to this subject comes from the theory of pattern formation in nature. Many physical phenomena giving rise to natural patterns can be understood in terms of the interaction of a short-range self-enhancing reaction and a long-range antagonistic reaction. Take a fire, for example. It is a self-enhancing process: more heat is released as more fuel is burned. In the process oxygen and fuel which act as antagonistic factors are consumed and this may lead to a fire's extinction if fuel is not replenished. Also, the heat produced is transported from its local source through diffusion. Thus, we have the two main ingredients for pattern formation, namely, a local antagonistic interaction between two species (or reactions) coupled with a means of transport of their products. Historically, this is also one of the first examples of reaction-diffusion systems

studied scientifically, for obvious reasons given the necessity for improved heating and lighting at the beginning of the industrial age. In his "Christmas Lectures" at the Royal Society in London, Michael Faraday discussed the importance of understanding the candle flame and its analogy with the process of respiration of biological organisms (Faraday, 1861). The flame of the candle is an archetypical nonlinear reaction-diffusion system that today, after decades of research, provides a basis for the science of combustion. In this article, we review the essential topics in the field of reaction-diffusion systems from a theoretical point of view and also consider some of their numerous applications.

2. Theoretical Aspects

A reaction-diffusion (RD) equation is typically obtained by combining Fick's law of diffusion with the chemical reaction rate law. Although the theory can be made rigorous by using the theory of stochastic differential equations leading to the Fokker-Planck equation (Øksendal, 2003), we present here a heuristic argument. If we consider for simplicity a small domain interval on the line inside which we have a concentration c of some reacting species, then the diffusive flux J_{in} of c into one side of the small region will depend on the concentration gradient, $\partial c / \partial x$, at that boundary and the diffusion coefficient, D, with

$$J_{in} = -D \left(\partial c / \partial x \right)_{in}$$

The parameter $D > 0$ is called diffusivity with physical units of m^2 / s. The diffusive flux out of the region at the other side J_{out} will similarly be given by

$$J_{out} = -D \left(\partial c / \partial x \right)_{out}$$

,

where the concentration gradient is now evaluated at the other boundary. The rate at which the concentration grows due to diffusion then depends on the difference between these two fluxes and so involves the second derivative $\partial^2 c / \partial x^2$. If we add a kinetic reaction rate term $r(c)$, then the reaction-diffusion equation, which gives the rate of change of the concentration c in time at any spatial point, has the general form

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} + r(c) \qquad (1)$$

Some problems related to population dynamics, competition between species and chemistry lead to a system of RD equations (RD system) of the form

$$\begin{cases} \frac{\partial u}{\partial t} = D_1 \frac{\partial^2 u}{\partial x^2} + f(u, v) \\ \frac{\partial v}{\partial t} = D_2 \frac{\partial^2 v}{\partial x^2} + f(u, v) \end{cases} \qquad (2)$$

From a mathematical point of view, systems of equations such as (2) must be well posed in order to exhibit appropriate solutions. The problem is fully specified once appropriate initial conditions

$$u(x,0) = u_0(x) \quad \text{and} \quad v(x,0) = v_0(x) \qquad (3)$$

are known. For an IVP (initial-value problem), one naturally asks whether there are solutions. In the case of reaction-diffusion systems, there are two different aspects to consider : local existence and global existence of the solutions. By local existence we mean the existence of the solutions over a short time interval. Global existence properties are exhibited by the solutions of the IVP when they are known to exist for all positive time.

These questions are difficult to deal with in general for RD systems although there is a well-developed body of results available in the literature (Grindrod, 1996).

Moreover, even if the existence of a particular type of solution is established, further important theoretical questions involve the uniqueness of the solution and the stability of this solution to small perturbations.

3. A chemical application

A simple archetypical example for a RD system is a cubic autocatalytic reaction between two chemicals according to the rule $A + B \rightarrow 2B$ with rate $r = \rho a b^2$.

Denoting by u the concentration of A and by v that of B, the two species satisfy the equations:

$$\begin{cases} \frac{\partial u}{\partial t} = D_A \frac{\partial^2 u}{\partial x^2} - \rho u v^2 \\ \frac{\partial v}{\partial t} = D_B \frac{\partial^2 v}{\partial x^2} + \rho u v^2 \end{cases} \qquad (4)$$

In system (4) D_A and D_B are the constant diffusion rates of A and B, respectively. We are interested in exact solutions to system (4). To simplify the calculations, we first make the transformations

$$x \rightarrow \sqrt{\frac{\rho}{D_A}} x, \quad t \rightarrow \rho t \qquad (5)$$

to obtain the system

$$\begin{cases} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - u v^2 \\ \frac{\partial v}{\partial t} = D \frac{\partial^2 v}{\partial x^2} + u v^2 \end{cases} \qquad (6)$$

where $D = \dfrac{D_B}{D_A}$.

Suppose that functions $U = U(x,t)$ and $V = V(x,t)$ are solutions to system (6). Then functions

$$u = U\left(\sqrt{\frac{\rho}{D_A}} x, \ \rho t\right) \text{ and } v = V\left(\sqrt{\frac{\rho}{D_A}} x, \rho t\right)$$

will be solutions to original system (4). In other words, if we know a solution to system (6), then we simply replace

x with $\sqrt{D_A/\rho} \, x$ and t with t/ρ to obtain a solution to system (4). For this reason, it suffices to solve system (6).

4. Exact solutions to the proposed model

We seek solutions to system (6) in the traveling wave

$$U(x, t) = a_0 + a_1 \tanh(k(x - \lambda t)) \qquad (7)$$

$$V(x, t) = b_0 + b_1 \tanh(k(x - \lambda t)) \qquad (8)$$

Substituting expressions (7) and (8) into system (6) we obtain an algebraic system of two polynomial equations in the variable $z = \exp(k(x - \lambda t))$. Equating the coefficients of z^i ($i = 0, 1, 2, \dots$) in each equation to zero, we obtain an algebraic system. Solving it we obtain following solution:

$$a_0 = b_1, \ a_1 = -b_1, \ b_0 = b_1, \ b_1 = b_1,$$

$$k = -b_1 / \sqrt{2}, \lambda = \sqrt{2} b_1, \ D = 1.$$

The value of b_1 may be arbitrary, that is, b_1 is a free real or complex parameter, say $b_1 = b$. Thus, a solution (U, V) to system (6) with $D = 1$ is given by

$$U(x,t) = b\left(1 + \tanh\left(\frac{\sqrt{2}b}{2}(x - \sqrt{2}bt)\right)\right) \qquad (9)$$

$$V(x,t) = b\left(1 - \tanh\left(\frac{\sqrt{2}b}{2}(x - \sqrt{2}bt)\right)\right) \qquad (10)$$

We conclude that when $D_A = D_B = \delta$ functions u and v given by

$$u = u(x, t) = b(1 + \tanh\xi),$$
$$v = v(x, t) = b(1 - \tanh\xi), \qquad (11)$$
$$\xi = \xi(x, t) = \frac{\sqrt{2}b}{2}\left(\sqrt{\frac{\rho}{\delta}} x - \sqrt{2}\rho b t\right).$$

are solutions to system (4).

Let $b > 0$. Observe that $0 < u < 2b$ and $0 < v < 2b$ for any x and t. The graphics of functions u and v given by (11) are shown in Figure 1 over the domain $-6 \leq x \leq 6$ and $0 \leq t \leq 1$. Observe that the corresponding surfaces meet in the three dimensional space through the line

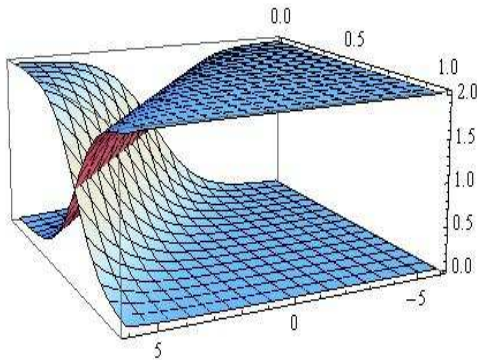$$\sqrt{\frac{\rho}{\delta}}\,x - \sqrt{2}\,\rho b t = 0.$$

Figure 1. Graphics of u and v given by (11) for $b = 1$, $\delta = 10$ and $\rho = 5$.

On the other hand, for a fixed $x_0 > 0$, curves

$$f(t) = u(x_0, t) \text{ and } g(t) = v(x_0, t)$$

meet at $t = \dfrac{x_0}{\sqrt{2\delta\rho\,b}}$. We illustrate this fact in Figure 2.
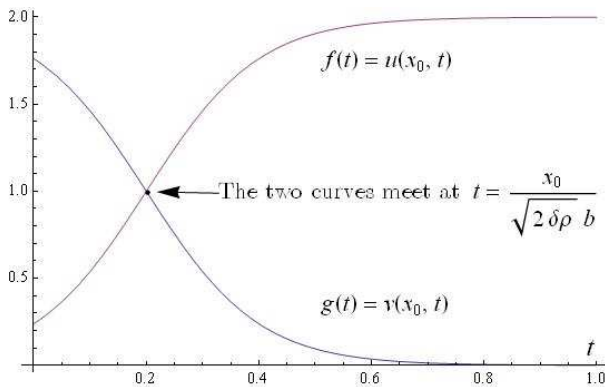

Figure 2.

2. Conclusions.

We have obtained exact solutions for a cubic autocatalytic reaction between two chemicals in the case when their constant diffusion rates coincide. The obtained expressions are relatively simple and allow simulating the associated chemical process. An open question is: are there exact solutions in the case when the diffusion rates are different?

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