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Computational Study of Traveling Wave Solutions of Isothermal Chemical Systems

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Abstract. This article studies propagating traveling waves in a class of reaction-diffusion systems which model isothermal autocatalytic chemical reactions as well as microbial growth and competition in a flow reactor. In the context of isothermal autocatalytic systems, two different cases will be studied. The first is autocatalytic chemical reaction of order m without decay. The second is chemical reaction of order m with a decay of order n, where m and n are positive integers and $m>n\geq 1$. A typical system in autocatalysis is $A+2B\to 3B$ and $B\to C$ involving two chemical species, a reactant A and an auto-catalyst B and C an inert chemical species.

The numerical computation gives more accurate estimates on minimum speed of traveling waves for autocatalytic reaction without decay, providing useful insight in the study of stability of traveling waves.

For autocatalytic reaction of order $m=2$ with linear decay $n=1$, which has a particular important role in chemical waves, it is shown numerically that there exist multiple traveling waves with 1, 2 and 3 peaks with certain choices of parameters.

AMS subject classifications: 34C20, 34C25, 92E20

Key words: Isothermal chemical systems, microbial growth in a flow reactor, traveling wave, multiple peak solutions, minimum speed, existence, non-existence.

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1 Introduction

In this paper we study two reaction-diffusion systems of the form

$$(I)\begin{cases} u_t=D_A u_{xx}-f(u,v), \\ v_t=D_B v_{xx}+f(u,v)-L(v), \end{cases} \tag{1.1}$$

and

$$(II)\begin{cases} u_t=D_A u_{xx}-f(u,v), \\ v_t=D_B v_{xx}+f(u,v), \end{cases} \tag{1.2}$$

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where f is a C^1 function defined on $[0,\infty)\times[0,\infty)$, L a C^1 function defined on $[0,\infty)$ with properties

$$f(u,0)=f(0,v)=0, \quad \text{and} \quad f(u,v)>0 \quad \text{on} \quad (0,\infty)\times(0,\infty),$$
$$L(0)=0 \quad \text{and} \quad L(v)>0 \quad \text{on} \quad (0,\infty),$$

and D_A, D_B are positive constants representing the diffusion coefficients of two different species, which are in general unequal due to different molecular weights and/or sizes.

The particular feature we are interested in is (i) the existence of multiple traveling waves for (1.1), and estimate of minimum speed for (1.2). Without loss of generality, we shall assume in what follows that $D_A=1$ and use d in place of D_B, since the general case can be transformed to this one by a simple non-dimensional scaling.

Many interesting phenomena in population dynamics, bio-reactors and chemical reactions can be modeled by a system of the form as in (1.1). For example, a system modeling microbial growth and competition in a flow reactor was first studied in [2] and [23], where a special case is $f(u,v)=F(u)v$, $L(v)=Kv$, K a positive constant, and $F(0)=0$ and $F'(0)>0$. In that context, u is the density of nutrient and v the density of microbial population. $L(v)$ is the death rate of microbial. Subsequent works with emphasis on traveling waves appeared later in [14] and [24].

Another interesting case arises from isothermal autocatalytic chemical reaction between two chemical spices A and B taking the form:

$$A+mB\longrightarrow(m+1)B \qquad \text{with rate } r[A][B]^m,$$

where $m\geq 1$ is an integer and $r>0$ is a rate constant. In that situation, $f(u,v)=uv^m$ with u the concentration density of A and v the density of B. If there is no decay, then $L(v)=0$. The resulting system is

$$(III)\begin{cases} u_t=u_{xx}-uv^m, \\ v_t=dv_{xx}+uv^m, \end{cases} \tag{1.3}$$

after a simple non-dimensional transformation. The importance of autocatalytic chemical reaction in chemical waves, Turing pattern formation and real-world chain chemical reactions is well documented in literature. The global dynamics of the Cauchy problem of (1.3) was studied in [3,16,19,20] in one and two dimensional cases using Renormalization Group method coupled with key a priori estimates. The existence and non-existence, as well as stability of traveling waves of (1.3) were investigated in [4–6,17]. In particular, it was established in [4] that for any fixed boundary value of $(u,v)=(0,a_0)$, $a_0>0$, at $-\infty$, there exists $C_*=C_*(d,a_0,m)$ such that there exists a traveling wave with speed C when $C\geq C_*$. That is, the situation is in the classical mono-stable category.

The traveling wave problem for (I) is far more complex. For example, the system

$$\begin{cases} u_t=u_{xx}-uv^m, \\ v_t=dv_{xx}+uv^m-kv^m, \end{cases} \tag{1.4}$$