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A Numerical Analysis Approach For Estimating The Minimum Traveling Wave Speed For An Autocatalytic Reaction

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A NUMERICAL ANALYSIS APPROACH FOR ESTIMATING THE MINIMUM TRAVELING WAVE SPEED FOR AN AUTOCATALYTIC REACTION

by

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ABSTRACT

This thesis studies the traveling wavefront created by the autocatalytic cubic chemical reaction A + 2B → 3B involving two chemical species A and B, where A is the reactant and B is the auto-catalyst. The diffusion coefficients for A and B are given by D_A and D_B. These coefficients differ as a result of the chemical species having different size and/or weight. Theoretical results show there exist bounds, v_* and v^*, depending on D_B / D_A, where for speeds $v \geq v^*$, a traveling wave solution exists, while for speeds $v < v_*$, a solution does not exist. Moreover, if $D_B \leq D_A$, v_* and v^* are similar to one another and in the order of D_B / D_A when it is small. On the other hand, when $D_A \leq D_B$ there exists a minimum speed v_{min}, such that there is a traveling wave solution if the speed $v > v_{min}$. The determination of v_{min} is very important in determining the dynamics of general solutions. To fill in the gap of the theoretical study, we use numerical methods to determine v_{min} for various cases. The numerical algorithm used is the fourth-order Runge-Kutta method (RK4).

This thesis is dedicated to my mother, Terry Urbanski, whose gracious support in all facets of my life made it possible for me to change careers and pursue a Master's degree in Mathematics. I am eternally grateful to her; to my father and his wife, John and Janet Blanken, whom I am tremendously thankful for, as they rearranged their lives to provide loving care for Logan while I went to work, school, and then studied, as well as being encouraging, supportive parents; to my grandfather, John Blanken (1924 – 2000), a mechanical engineer on the *Saturn V*, who instilled in me an appreciation for science and mathematics at a young age; to Ron Stopa, for being a warmhearted, adoring father to Logan and for his continuous support in my endeavors; to each of my family members, who provided me with encouragement during graduate school; to the greatest friend and study mate one could have, Victor Pareja. After taking seven classes together over five semesters at 15 weeks each, we had 450 hours of mathematically stimulating conversations during our 150 commutes, 187.5 hours of arduous classes, and 750 hours of cooperative learning, all for a grand total of 1,387.5 hours we spent together over a mere 17.5 months. Considering our chairman introduced us a week before we embarked on our mission, that is some intense "getting to know you" time; to Frank Lombardo, Vice President of Academic Affairs at Daytona Beach College (DBC), and Marc Campbell, Chair of the Mathematics Department at DBC, for the opportunity to become a DBC faculty member, which was and is my goal and dream; to the entire Mathematics Department at DBC for the warmth they provided during the past four years, thank you for welcoming me to the DBC family; to my son, Logan, who is the littlest and most special boy in my world. I look forward to playing "cars" with you.

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CHAPTER ONE: INTRODUCTION

Consider a specific case of the general isothermal autocatalytic system, $A + nB \rightarrow (n+1)B$, where $n = 2$, which is the cubic autocatalytic step:

$$A + 2B \rightarrow 3B \text{ with the rate } kab^2 \text{ and } k > 0.$$

Here, a is the concentration of the reactant A, and b is the concentration of the autocatalyst B. The cubic autocatalytic step has been used successfully in models of actual chemical reactions according to Billingham and Needham [2]. For example, according to Saul and Showalter [9], the cubic autocatalytic step is an agreeable model for the iodate-arsenous acid reaction and according to Gowland and Stedman [4], the xylamine-nitrate reaction.

Models of autocatalytic systems make an appearance in the field of Epidemiology, e.g. a is the concentration of a healthy population and b is the concentration of an infected population according to Bailey [1]. A diffusion coefficient, D, is introduced, which is the ratio of the diffusion rate of the autocatalyst to that of the reactant, (i.e. D_B/D_A). D can vary greatly depending upon the mobility of the infected population and/or disease. Moreover, D can be significantly different from unity. (Billingham and Needham, [2]). Given a fixed set of initial conditions, it is this D that may cause the minimum speed, v_{min}, to vary.

Experiments indicate the existence of traveling wave fronts in chemical systems where the cubic catalysis is a key step according to Saul and Showalter [9], as well as Zaikin and Zhabotinski [10]. A result of the interaction of two different chemical species is wave fronts or traveling waves. According to Chen and Qi [3], Hanna, Saul and Showalter [9], and Merkin and Needham [6], given the uniform concentration of a reactant and the local introduction of an autocatalyst, it has been witnessed that the reaction creates wave fronts as the reactant is consumed by the autocatalyst, ahead of the wave fronts. These wave fronts move outward, away from the initial reaction zone. In the end there is the non-uniform distribution of chemical species. The phenomenon of the wave front or traveling wave will be studied in this thesis.

1.1 A Dimensionless System

Consider the standard partial differential equations that govern the mass concentration/molecular diffusion for this cubic reaction scheme:

$$\frac{\partial a}{\partial t} = D_A \frac{\partial^2 a}{\partial x^2} - kab^2; \quad \frac{\partial b}{\partial t} = D_B \frac{\partial^2 b}{\partial x^2} + kab^2 \tag{1.1}$$

where kab^2 is the kinetic portion and D_A and D_B are the diffusion rates of *A* and *B*, respectively.

Experimental setups dictate the initial conditions as follows:

$$a(x,0) = a_0, \qquad b(x,0) = g(x) \qquad\qquad \forall\ x \in \mathbb{R}$$

where the positive constant a_0 represents the uniform distribution of the reactant and $g(x)$ is a non-negative function with compact support, meaning that support of $g(x) = \overline{\{x \mid g(x) > 0\}}$.

Now we introduce the dimensionless parameters for the dependent and independent variables:

$$D = \frac{D_B}{D_A}, \qquad \overline{a} = \frac{a}{a_0}, \qquad \overline{b} = \frac{b}{a_0}, \qquad \overline{t} = ka_0^2 t, \qquad \overline{x} = x\sqrt{\frac{ka_0^2}{D_A}}, \qquad g = \frac{g}{a_0}.$$

Thus,

$$a(x,t) = a_0 \overline{a}(\overline{x}, \overline{t})$$

and ,

$$b(x,t) = a_0 \overline{b}(\overline{x}, \overline{t}).$$

Moreover,

$$\frac{\partial a}{\partial t} = \frac{\partial a(x,t)}{\partial t} = a_0 \frac{\partial \overline{a}(\overline{x}, \overline{t})}{\partial t} = a_0 \frac{\partial \overline{a}}{\partial \overline{t}} \frac{d\overline{t}}{dt} = ka_0^3 \frac{\partial \overline{a}}{\partial \overline{t}}, \qquad \text{where} \quad \frac{d\overline{t}}{dt} = ka_0^2$$

also,

$$\frac{\partial a}{\partial x} = \frac{\partial a(x,t)}{\partial x} = a_0 \frac{\partial \overline{a}(\overline{x}, \overline{t})}{\partial x} = a_0 \frac{\partial \overline{a}}{\partial \overline{x}} \frac{d\overline{x}}{dx} = a_0 \frac{\partial \overline{a}}{\partial \overline{x}} \sqrt{\frac{ka_0^2}{D_A}}, \qquad \text{where} \quad \frac{d\overline{x}}{dx} = \sqrt{\frac{ka_0^2}{D_A}}$$

and

$$\frac{\partial^2 a}{\partial x^2} = a_0 \frac{\partial}{\partial \bar{x}}\left(\frac{\partial \bar{a}}{\partial \bar{x}}\right) = a_0 \frac{\partial}{\partial \bar{x}}\left(\frac{ka_0^2}{D_A}\right)^{\frac{1}{2}} = a_0\left(\frac{ka_0^2}{D_A}\right)^{\frac{1}{2}}\left(\frac{ka_0^2}{D_A}\right)^{\frac{1}{2}}\frac{\partial^2 \bar{a}}{\partial \bar{x}^2} = \frac{ka_0^3}{D_A}\frac{\partial^2 \bar{a}}{\partial \bar{x}^2}.$$

The equivalent partials for $b(x,t)$ are

$$\frac{\partial b}{\partial t} = \frac{\partial b(x,t)}{\partial t} = a_0 \frac{\partial \bar{b}(\bar{x},\bar{t})}{\partial t} = a_0 \frac{\partial \bar{b}}{\partial \bar{t}}\frac{d\bar{t}}{dt} = ka_0^3 \frac{\partial \bar{b}}{\partial \bar{t}}, \quad \text{where } \frac{d\bar{t}}{dt} = ka_0^2$$

$$\frac{\partial b}{\partial x} = \frac{\partial b(x,t)}{\partial x} = a_0 \frac{\partial \bar{b}(\bar{x},\bar{t})}{\partial x} = a_0 \frac{\partial \bar{b}}{\partial \bar{x}}\frac{d\bar{x}}{dx} = a_0 \frac{\partial \bar{b}}{\partial \bar{x}}\sqrt{\frac{ka_0^2}{D_A}}, \quad \text{where } \frac{d\bar{x}}{dx} = \sqrt{\frac{ka_0^2}{D_A}}$$

and

$$\frac{\partial^2 b}{\partial x^2} = a_0 \frac{\partial}{\partial \bar{x}}\left(\frac{\partial \bar{b}}{\partial \bar{x}}\right) = a_0 \frac{\partial}{\partial \bar{x}}\left(\frac{ka_0^2}{D_A}\right)^{\frac{1}{2}} = a_0\left(\frac{ka_0^2}{D_A}\right)^{\frac{1}{2}}\left(\frac{ka_0^2}{D_A}\right)^{\frac{1}{2}}\frac{\partial^2 \bar{b}}{\partial \bar{x}^2} = \frac{ka_0^3}{D_A}\frac{\partial^2 \bar{b}}{\partial \bar{x}^2}.$$

Note that $D_B = DD_A$. We remove bars, make the appropriate substitutions into (1.1), and simplify, to obtain the following dimensionless initial value problem (IVP):

$$\frac{\partial a}{\partial t} = \frac{\partial^2 a}{\partial x^2} - ab^2, \; x \in \mathbb{R}, t > 0$$

$$\frac{\partial b}{\partial t} = D\frac{\partial^2 b}{\partial x^2} + ab^2, \; x \in \mathbb{R}, t > 0$$

$$a(x,0) = 1, \quad b(x,0) = g(x) \quad \text{for } x \in \mathbb{R}, t = 0. \tag{1.2}$$

The emphasis of this paper will be given when $D \neq 1$, which occurs when the chemical substances involved have different molecular weights and/or sizes.

1.2 Ordinary differential equations (ODE) system for Traveling Wave Solution

The phenomenon of propagating wave fronts corresponds to (1.2), where there are two traveling wave fronts expanding outwards to $\pm\infty$, both moving at a certain speed, *v*, according to Chen and Qi [3] and

Zaikin and Zhabotinskii [10]. We consider the wave front approaching positive infinity and make the following change of variables $z = x - vt$, thus $(a(x,t), b(x,t)) = (\alpha(z), \beta(z))$. We transform (1.2) using the aforementioned change of variables, which that requires the following partial derivatives:

$$\frac{\partial a}{\partial t} = \frac{\partial \alpha}{\partial z}\frac{dz}{dt} = \alpha_z(-v) = -v\alpha_z, \quad \text{and}$$

$$\frac{\partial b}{\partial t} = \frac{\partial \beta}{\partial z}\frac{dz}{dt} = \beta_z \cdot (-v) = -v\beta_z$$

as well as

$$\frac{\partial^2 a}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial a}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial a}{\partial z}\frac{dz}{dt}\right) = \frac{\partial}{\partial x}\left(\alpha_z \cdot 1\right) = \frac{\partial}{\partial x}\left(\alpha_z\right) = \alpha_{zz},$$

and

$$\frac{\partial^2 b}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial \beta}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial \beta}{\partial z}\frac{dz}{dt}\right) = \frac{\partial}{\partial x}\left(\beta_z \cdot 1\right) = \frac{\partial}{\partial x}\left(\beta_z\right) = \beta_{zz}.$$

We substitute the four partial derivatives into (1.2), which gives the following system of ODEs:

$$\begin{gathered} \alpha_{zz} + v\alpha_z = \alpha\beta^2 \\ D\beta_{zz} + v\beta_z = -\alpha\beta^2 \\ \lim_{z\to\infty}(\alpha(z), \beta(z)) = (1,0) \\ \lim_{z\to-\infty}(\alpha(z), \beta(z)) = (0,1). \end{gathered} \tag{1.3}$$

The constant traveling wave speed, *v*, is greater than zero.

The organization of the paper is as follows: Chapter Two lists the theorems from Chen and Qi [3], Chapter Three contains a preliminary analysis and Chapters Four and Five discuss the cases of $D \geq 1$ and $D < 1$, respectively. The material in Chapters One through Five originated from the work of Dr. Yuan-wei Qi and Dr. Xinfu Chen presented in their paper "*Sharp Estimates on Minimum Traveling Wave Speed of Reaction Diffusion Systems Modeling Auto-Catalysis*" [3]. Chapter Six describes the numerical analysis used to determine the minimum speeds for both small and large D, which was completed in this thesis with the guidance of Dr. Yuan-wei Qi. Chapter Seven demonstrates the results of the numerical analysis.

CHAPTER TWO: THE TRAVELING WAVE PROBLEM

The traveling wave problem for $v > 0$ is to find $(\alpha, \beta) \in \left[C^2(\mathbb{R})\right]^2$ that satisfies the ODE system (1.3). The existence and non-existence of a traveling wave solution will be studied. Moreover, we want to estimate the minimum speed for the traveling wave speed (i.e., with respect to the diffusion coefficient ratio, *D*, for what range of *v* does a traveling wave solution exist).

Previous studies by Billingham and Needham [2] concluded that a traveling wave solution exists if $v \geq 2\sqrt{D}$. Furthermore, results by Qi [7] improved the work of Billingham and Needham [2] with a more detailed study for system (1.3), that is there is a traveling wave solution when:

$$v \geq \sqrt{2D-1} \quad \text{when } D \geq 1 \text{ and}$$

$$v \geq \sqrt{D} \quad \text{when } D < 1$$

and there is not a traveling wave solution when:

$$v \leq \frac{\sqrt{D}}{6} \quad \text{when } D \geq 1 \text{ and}$$

$$v \leq \frac{D}{\sqrt{6}} \quad \text{when } D < 1.$$

It is also known that:

$$v_{\min} = \frac{1}{\sqrt{2}} \quad \text{when } D = 1.$$

Presented here is a good estimate for $v_{\min}$, for both small and large *D*. In addition, the gap between the general case and the case of $D = 1$ will be closed.

2.1 The Case of $D < 1$

The main result of Chen and Qi [3] for the case of $D < 1$ is:

Theorem 1: *Suppose D < 1. For the traveling wave problem presented in equation (1.3), there exists a unique solution (up to translation) if $v \ge \frac{4D}{\sqrt{1+4D}}$; there does not exist any solution if $v < \frac{D}{\sqrt{2}}$.*

Their results are much better than the previous works.

2.2 The Case of $D \ge 1$

The main result of Chen and Qi [3] for the case of $D \ge 1$ is:

Theorem 2: *Suppose $D \ge 1$. There exists a positive constant $v_{\min}$ such that (1.3) admits a solution if and only if $v \ge v_{\min}$. In addition, $v_{\min}$ satisfies the estimate*

$$\sqrt{\frac{D}{2}} \le v_{\min} \le \sqrt{\frac{D}{1+1/D}}.$$

As was the case for $D < 1$, the result by Chen and Qi [3] for $D \ge 1$ was a great improvement on previous works.

Theorems 3 and 4 are the results of Chen and Qi [3] that not only apply to the special case of the cubic autocatalytic reaction step, but also the general case. Recall that the general isothermal autocatalytic chemical reaction with order $n \ge 1$ is $A + nB \to (n+1)B$ with rate kab^n. Similar to the equations in (1.2), the dimensionless IVP is:

$$\begin{aligned}
&\frac{\partial a}{\partial t} = \frac{\partial^2 a}{\partial x^2} - ab^n, && x \in \mathbb{R}, t > 0 \\
&\frac{\partial b}{\partial t} = D\frac{\partial^2 b}{\partial x^2} + ab^n, && x \in \mathbb{R}, t > 0 \\
&a(x,0) = 1, \quad b(x,0) = g(x), && x \in \mathbb{R}, t = 0.
\end{aligned} \tag{2.1}$$

By making the same argument and change of variables as in §1.2, that is $z = x - vt$, thus $(a(x,t), b(x,t)) = (\alpha(z), \beta(z))$ and so system (2.1) becomes:

$$\alpha_{zz} + v\alpha_z = \alpha\beta^n$$

$$D\beta_{zz} + v\beta_z = -\alpha\beta^n$$

$$\lim_{z\to\infty}(\alpha(z), \beta(z)) = (1,0)$$

$$\lim_{z\to-\infty}(\alpha(z), \beta(z)) = (0,1)$$

(2.2)

for all real values of *z*.

<u>2.3 The Case of *D* < 1 and *n* ≥ 1</u>

<u>Theorem 3:</u> *Suppose D < 1 and $n \geq 2$. A unique (up to translation) traveling wave solution exists for (2.2) if $v \geq \frac{4D}{\sqrt{1+4D}}$. On the other hand, there exists no solution for (2.2) if $v < \frac{D}{\sqrt{K(n)}}$, where K(n) is a constant, which increases with n. In particular, K(1) = ¼, K(2) = 2.*

<u>2.4 The Case of *D* ≥ 1 and *n* ≥ 1</u>

<u>Theorem 4</u>: *Suppose $D \geq 1$ and $n \geq 1$. There exists a positive constant v_{min} such that (2.2) admits a traveling wave is and only if $v \geq v_{min}$. In addition, v_{min} is bounded by*

$$\sqrt{\frac{D}{K(n)}} \leq v_{min} \leq \sqrt{\frac{D}{K(n)}} \frac{1}{\sqrt{1-(1-\frac{1}{D})\frac{\sqrt{4K(n)+1}-1}{\sqrt{4K(n)+1}+1}}}$$

where K(n) is the same constant as in Theorem 3.

CHAPTER THREE: EXISTENCE AND PROPERTIES OF THE TRAVELING WAVE

Consider the traveling wave equation of unit speed:

$$u_{zz} + u_z = ku(1-u)^n,\ u \in [0,1] \text{ on } \mathbb{R} \text{ with } u(-\infty) = 0 \text{ and } u(\infty) = 1. \tag{3.1}$$

This resembles equation (2.2) for the case $D = 1$. Here $n \geq 1$ is a parameter and k is a positive constant.

It is easy to verify that if a solution exists, it satisfies $u_z > 0$ on $\mathbb{R}$. Let u be the independent variable, then using the change of variables

$$u_z = Q(u) = Q$$

then

$$u_{zz} = \frac{dQ}{dz}(u) = \frac{dQ}{du}\frac{du}{dz} = Q'Q = QQ'.$$

Thus equation (3.1) becomes

$$QQ' + Q = ku(1-u)^n, \quad u \in [0,1]$$

$$Q(0) = 0 \text{ and } Q(u) > 0. \tag{3.2}$$

Note: A traveling wave solution must satisfy $Q(1) = 0$.

<u>3.1 Existence</u>

<u>*Lemma 1:*</u> *For each $n \geq 1$ and $k > 0$, there exists a unique solution $Q = (n,k;\cdot)$ to (3.2). In addition, there exists a positive constant $K(n)$ such that $Q = (n,k;1) = 0$ if $k \in (0, K(n)]$ and $Q = (n,K;1) > 0$ if $k \in (K(n), \infty)$. Consequently, (3.2) admits a solution if and only if $k \in (0, K(n)]$. $K(n)$ is a strictly increasing function of n and K(1) = $\frac{1}{4}$, K(2)=2.*

__Proof:__ We want to show that for $k_1 > k_2$, $Q_1(u) > Q_2(u)$ when $0 < u << 1$.

Let $k_1 > k_2$; $Q_1(u) = Q_1(n,k_1;u)$ and $Q_2(u) = Q_2(n,k_2;u)$. When $0 < u << 1$, suppose $Q_1(u) \approx c_1 u$ and $Q_2(u) \approx c_2 u$, where c_1, c_2 are constants. From (3.2) for $Q_1(n,k_1;u)$

$$Q_1 Q_1' + Q_1 = k_1 u(1-u)^n.$$

Substituting $c_1 u$ for $Q_1(n,k_1;u)$ gives us

$$(c_1 u)c_1 + c_1 u \approx k_1 u(1-u)^n$$

thus,

$$c_1^2 + c_1 - k_1 = 0.$$

Because $Q_1(u) > 0$ and $u > 0$, thus

$$c_1 = \frac{-1 + \sqrt{1 + 4k_1}}{2}.$$

Similarly,

$$c_2 = \frac{-1 + \sqrt{1 + 4k_2}}{2}.$$

Since $k_1 > k_2$, then

$$c_1 > c_2.$$

Thus,

$$Q_1(u) > Q_2(u) \text{ when } 0 < u << 1.$$

■

Next we show that $Q_1(u) > Q_2(u)$ in $(0,1)$. Suppose the contrary, then $\exists\, u_0 \in (0,1)$ such that $Q_2(u_0) = Q_1(u_0)$. From above, we have seen that when $0 < u << 1$, $Q_1(u) > Q_2(u)$. Therefore, $Q_1'(u_0) \le Q_2'(u_0)$. Consequently, at $u = u_0$ this must hold:

$$Q_1 Q_1\,'(u) + Q_1(u) \le Q_2 Q_2\,'(u) + Q_2(u)$$

but

$$Q_1 Q_1\,' + Q_1 = k_1 u(1-u)^n > Q_2 Q_2\,' + Q_2 = k_2 u(1-u)^n.$$

This is a contradiction. Thus

$$Q_1\left(u\right) > Q_2(u) \text{ in the interval } (0,1).$$

In consequence, if $Q(n,k_1;1) = 0$, then $Q(n,k_2;1) = 0$ for all $k_1 < k_2$ and if $Q(n,k_2;1) > 0$ then $Q(n,k_1;1) > 0$ for all $k_1 > k_2$.

■

<u>3.2 Properties</u>

Suppose (v,α,β) solves (2.2), then

$$[\alpha_z + v\alpha + D\beta_z + v\beta]_z = 0$$

and thus the expression within brackets is a constant function. Applying the boundary conditions gives the following equation:

$$\alpha_z + D\beta_z + v(\alpha + \beta - 1) = 0, \quad \forall\ z \in \mathbb{R}.$$

Introducing $w = \beta_z$, the system of equations (2.2) is equivalent to:

$$\alpha_z = v(1-\alpha-\beta) - Dw$$

$$\beta_z = w$$

$$w_z = -D^{-1}(\alpha\beta^n + vw)$$

$$\lim_{z\to\infty}(\alpha(z),\beta(z),w(z)) = (1,0,0)$$

$$\lim_{z\to-\infty}(\alpha(z),\beta(z),w(z)) = (0,1,0).$$

(3.3)

<u>Proposition 1:</u> *The systems (2.2) and (3.3) are equivalent. Any solution* (α,β) *to (2.2) or* (α,β,w) *to (3.3) has the following properties:*

1. $\alpha_z > 0 > \beta_z$, on $\mathbb{R}$
2. *(a)* $\alpha+\beta<1$ *on* $\mathbb{R}$ *if* $D<1$, *(b)* $\alpha+\beta\equiv 1$ *if* $D=1$, *and (c)* $\alpha+\beta>0$ *if* $D>1$
3. $v = \int_{-\infty}^{\infty}\alpha(z)\beta^n(z)dz > 0$
4. *The equilibrium point (0, 1, 0) of (3.2) is a saddle with a two-dimensional stable manifold and a one-dimensional unstable manifold. The eigenvalues and associated eigenvectors are:*

$$\lambda_1 = -vD^{-1}, \qquad \mathbf{e}_{\lambda_1} = (0,-1,-\lambda_1)^T$$

$$\lambda_2 = -\frac{1}{2}\left(\sqrt{v^2+4}+v\right), \quad \mathbf{e}_{\lambda_2} = \left[\lambda_2\left(D\lambda_2+v\right),-1,-\lambda_2\right]^T$$

$$\lambda_3 = \frac{1}{2}\left(\sqrt{v^2+4}-v\right), \quad \mathbf{e}_{\lambda_3} = \left[\lambda_3\left(D\lambda_3+v\right),-1,-\lambda_3\right]^T$$

5. *When n > 1, the equilibrium point (0,0,1) of (3.3) is degenerate; it has a two-dimensional stable manifold and a one-dimensional center manifold. The eigenvalues and associated eigenvectors are:*

$$\mu_1 = -v, \qquad \mathbf{e}_{\mu_1} = (1,0,0)^T$$

$$\mu_2 = -vD^{-1}, \quad \mathbf{e}_{\mu_2} = \left(0,1,-vD^{-1}\right)^T$$

$$\mu_3 = 0, \qquad \mathbf{e}_{\mu_3} = (1,-1,0)^T$$

<u>*Proof of (1):*</u> Consider $\alpha_z > 0$. We multiply the first equation of (2.2)

$$\alpha_{zz} + v\alpha_z = \alpha\beta^n$$

by e^{vz} and integrate on $(-\infty, z)$. We find that

$$e^{vz}\alpha_z = \int_{-\infty}^{z} \alpha e^{vs}\beta^n ds.$$

Because $\alpha(z) > 0$ and $\beta(z) > 0$ for $-\infty < z < \infty$, then

$$\alpha_z = e^{-vz}\int_{-\infty}^{z} \alpha e^{vs}\beta^n ds > 0, \quad \forall\ z \in \mathbb{R}.$$

■

Next consider $\beta_z < 0$. We multiply the second equation of (2.2)

$$D\beta_{zz} + v\beta_z = -\alpha\beta^n$$

by $e^{vD^{-1}z}$ and integrate on $(-\infty, z)$. We find that

$$e^{vD^{-1}z}\beta_z = -\int_{-\infty}^{z} \alpha e^{vD^{-1}s}\beta^n ds.$$

Because $\alpha(z) > 0$ and $\beta(z) > 0$ for $-\infty < z < \infty$, then

$$\beta_z = -e^{-vD^{-1}z}\int_{-\infty}^{z} \alpha e^{vD^{-1}s}\beta^n ds < 0, \quad \forall z \in \mathbb{R}.$$

■

Proof of (2a):

The proof for (*2a*) is similar to the proof presented for (*2b*).

Proof of (2b): From (3.3), for $D = 1,$ we have

$$(\alpha_z + \beta_z) + v(\alpha + \beta) = v.$$

We multiply by e^{vz} and integrate, which results in the following

$$e^{vz}\left(\alpha + \beta\right) = e^{vz}.$$

Therefore, $\alpha + \beta \equiv 1$.

■

Proof (2c): Similarly, (*2c*) is true.

■

Proof of (3): From the first equation of (2.2)

$$\alpha_{zz} + v\alpha_z = \alpha\beta^n, \quad \forall z \in \mathbb{R}, \; a \geq 0.$$

We integrate from $\left(-\infty, \infty\right)$, thus

$$(\alpha_z + v\alpha)(\infty) - (\alpha_z + v\alpha)(-\infty) = \int_{-\infty}^{\infty} \alpha\beta^n dz.$$

Using the condition that $\alpha(\infty) = 1$, this implies $\alpha_z(\infty) = 0$ and $\alpha(-\infty) = 0$, then,

$$v = \int_{-\infty}^{\infty} \alpha(z)\beta^n(z)dz > 0.$$

■

Verification of (4): Since $\left(0,1,0\right)$ is an equilibrium point, then we have the following Jacobian matrix **M**:

$$\mathbf{M} = \begin{pmatrix} \frac{\partial f}{\partial \alpha} & \frac{\partial f}{\partial \beta} & \frac{\partial f}{\partial w} \\ \frac{\partial g}{\partial \alpha} & \frac{\partial g}{\partial \beta} & \frac{\partial g}{\partial w} \\ \frac{\partial h}{\partial \alpha} & \frac{\partial h}{\partial \beta} & \frac{\partial h}{\partial w} \end{pmatrix}_{at\ \left(0,1,0\right)} = \begin{pmatrix} -v & -v & -D \\ 0 & 0 & 1 \\ -D^{-1} & 0 & -D^{-1}v \end{pmatrix},$$

where $f = \alpha_z = v(1-\alpha-\beta) - Dw$, $g = \beta_z = w$, and $h = w_z = -D^{-1}(\alpha\beta^n + vw)$.

We determine the eigenvalues by solving $\det(\mathbf{M} - \lambda\mathbf{I}) = 0$, which gives us:

$$(-v-\lambda)(-\lambda)(-D^{-1}v-\lambda) + (-D^{-1})(-v-\lambda D) = 0.$$

This simplifies to

$$(-\lambda^2 - v\lambda + 1)(D^{-1}v + \lambda) = 0.$$

The three eigenvalues are

$$\lambda_1 = -vD^{-1}$$
$$\lambda_2 = -\frac{1}{2}(\sqrt{v^2+4} + v)$$
$$\lambda_3 = \frac{1}{2}(\sqrt{v^2+4} - v).$$

Case 1: $\lambda_1 = -vD^{-1}$,

$$(\mathbf{M} - \lambda\mathbf{I})\mathbf{x} = \begin{pmatrix} -v+vD^{-1} & -v & -D \\ 0 & vD^{-1} & 1 \\ -D^{-1} & 0 & -D^{-1}v + D^{-1}v \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \mathbf{0}.$$

This yields the following system of equations:

$$(-v+vD^{-1})x_1 + (-v)x_2 + (-D)x_3 = 0$$

$$vD^{-1}x_2 + x_3 = 0$$

$$-D^{-1}x_1 = 0.$$

Choose $x_2 = -1$, then

$$x_3 = vD^{-1} = -\lambda_1$$

and for $\lambda_1 = -vD^{-1}$

$$\mathbf{e}_{\lambda_1} = (0,-1,-\lambda_1)^T.$$

Similarly, when $\lambda_2 = -\frac{1}{2}(\sqrt{v^2 + 4} + v)$, the associated eigenvector is

$$\mathbf{e}_{\lambda_2} = \left[\lambda_2 \left(D\lambda_2 + v\right), -1, -\lambda_2\right]^T$$

and when $\lambda_3 = \frac{1}{2}(\sqrt{v^2 + 4} - v)$, the associated eigenvector is

$$\mathbf{e}_{\lambda_3} = (\lambda_3(D\lambda_3 + v), -1, -\lambda_3)^T.$$

■

Verification (5): The verification is similar to the fourth property of Proposition 1.

■

This completes the proof of Proposition 1.

Remark: The third property indicates that the speed is greater than zero, while the fourth property tells us the traveling wave is the one-dimensional unstable manifold, starting at the equilibrium point (0,1,0). Thus if a traveling wave exists for a speed, $v > 0$, it is unique, up to a translation.

3.3 Transforming System (3.3) to a Non-Autonomous 2 × 2 System

Next we transform the third order autonomous system (3.3) to a second order non-autonomous system. We use $u = 1 - \beta$ as the independent variable, which is acceptable since the solution we seek $\beta_z < 0$, thus $z \to 1 - \beta(z)$ has an inverse. Consider the following change of variables:

$$u = 1 - \beta, \qquad A = \frac{D\alpha}{v^2}, \qquad y = \frac{vz}{D}, \qquad \kappa = \frac{D}{v}$$

First we determine α_z:

$$\alpha = \frac{v^2}{D} A \Rightarrow \alpha_z = \frac{v^2}{D} A_z = \frac{v^2}{D} \frac{dA}{dz}$$

and then w:

$$w = \beta_z = \frac{d\beta}{dz} = \frac{d\beta}{du}\frac{du}{dz} = \frac{d\beta}{du}\frac{du}{dy}\frac{dy}{dz} = (-1)\frac{du}{dy}\left(\frac{v}{D}\right) = -\frac{v}{D}u_y.$$

From the first equation of (3.3)

$$\alpha_z = v(1-\alpha-\beta) - Dw\,,$$

using the above change of variables for α, β, α_z, and w, we have the following:

$$\frac{v^3}{D^2}A_y = v\left[1 - \frac{v^2}{D}A - (1-u)\right] - D\left(-\frac{v}{D}u_y\right).$$

This implies

$$A_y = -DA + \frac{D^2}{v^2}(u + u_y)$$

and therefore

$$A_y = \kappa^2(u + u_y) - DA \text{ on } \mathbb{R}. \tag{3.4}$$

Since,

$$\beta_z = w \quad \text{and} \quad w_z = -D^{-1}(\alpha\beta^n + vw)$$

then

$$w_z = \beta_{zz} = \frac{d^2\beta}{dz^2} = \frac{d}{dz}\left(\frac{d\beta}{dz}\right) = \frac{d}{dz}\left(-\frac{v}{D}u_y\right) = -\frac{v}{D}\left(\frac{d}{dz}\left(\frac{du}{dy}\right)\right) = -\frac{v}{D}\left(\frac{d^2u}{dy^2}\frac{dy}{dz}\right) = -\frac{v}{D}u_{yy}\frac{v}{D} = -\frac{v^2}{D^2}u_{yy}.$$

Substituting the expressions for w_z, α, β, and β_z into the third equation of (3.3)

$$w_z = -D^{-1}(\alpha\beta^n + vw)$$

we have:

$$-\frac{v^2}{D^2}u_{yy} = -D^{-1}\left[\frac{v^2}{D}A(1-u)^n - \frac{v^2}{D}u_y\right].$$

This simplifies to

$$u_{yy} + u_y = A(1-u)^n \text{ on } \mathbb{R}.$$

(3.5)

Since $u_y > 0$ for the solution sought, we can use u as the independent variable. Let $P(u) = u_y$ then

$$u_{yy} = \frac{d}{dy}\big(P(u)\big) = \frac{dP}{dy}(u) = \frac{dP}{du}\frac{du}{dy} = P'P = PP'.$$

Next consider

$$A_y = A(u)_y = \frac{dA}{dy} = \frac{dA}{du}\frac{du}{dy} = PA'.$$

Thus we have the system

$$PP' = A(1-u)^n - P, \quad \forall u \in [0,1]$$

$$PA' = \kappa^2(P+u) - DA, \quad \forall u \in [0,1]$$

$$P(u) > 0, \quad A(u) > 0, \quad \forall u \in (0,1)$$

$$P(0) = 0, \quad A(0) = 0.$$

(3.6)

since $u(-\infty) = 0$ and $u(\infty) = 1$. $A(u) > 0$ because $A = \dfrac{D\alpha}{v^2}$, where $D, v, \alpha > 0$.

This is an equivalent system of second order non-autonomous ODEs.

3.4 Unique Solution for the Non-Autonomous System

Lemma 2: *For every $D > 0$ and $\kappa > 0$, (3.6) admits a unique solution. In addition,*

$$P(u) = \lambda u + O(u^2)$$

$$A(u) = \lambda(1+\lambda)u + O(u^2), \quad D > 0$$

where $\lambda = \frac{1}{2}\left(\sqrt{4\kappa^2 + D^2} - D\right)$ *, the only positive root to* $\lambda(\lambda + D) = \kappa^2$.

Furthermore, $A'(u) > 0$ *for all* $u \in [0,1)$ *and there are only two possible cases:*

(a) $P(1) > 0;$ *∄ any traveling wave solution to (2.2)*

(b) $P(1) = 0;$ *∃ a traveling wave solution to (2.2) unique up to translation.*

<u>*Derivation:*</u> To derive $P(u) = \lambda u + O(u^2)$ and $A(u) = \lambda(1+\lambda)u + O(u^2)$ as $D > 0$, let $P(u) \approx c_1 u$ and $A(u) \approx l_2 u$. This implies

$$P'(u) \approx c_1 \text{ and } A'(u) \approx l_2.$$

Making the appropriate substitution for $P,\ P',\ \text{and}\ A$ into the first equation of (3.6) gives us

$$c_1^2 u \approx l_2 u(1-u)^n - c_1 u.$$

Since $u \to 0$ we have

$$c_1^2 + c_1 - l_2 = 0. \tag{3.7}$$

Solving (3.7) for c_1 gives us

$$c_1 = -\frac{1}{2} \pm \frac{1}{2}\sqrt{1 + 4l_2}.$$

Making the appropriate substitution for $P,\ A,\ \text{and}\ A'$ into the second equation of (3.6) gives us

$$(c_1 u)(l_2) = \kappa^2(c_1 u + u) - Dl_2 u$$

and thus

$$l_2(c_1 + D) = \kappa^2(c_1 + 1).$$

When $D = 1$, then $l_2 = \kappa^2$. When $D \neq 1$, consider $l_2 = c_1^2 + c_1$ from (3.7), which gives us

$$(c_1^2 + c_1)(c_1 + D) = \kappa^2(c_1 + 1).$$

Solving for c_1 gives us

$$c_1 = \frac{-D \pm \sqrt{D^2 + 4\kappa^2}}{2}. \tag{3.8}$$

Since $P(u) > 0$ for all $u \in (0,1)$ and we let $P(u) \approx c_1 u$, therefore we have

$$c_1 = \frac{1}{2}\left(\sqrt{D^2 + 4\kappa^2} - D\right) = \lambda,$$

the only positive root to $\lambda(\lambda + D) = \kappa^2$ and $P(u) = \lambda u + O(u^2)$. Since $c_1^2 + c_1 = l_2$, where $c_1 = \lambda$, thus

$$l_2 = \lambda(\lambda + 1) \text{ and } A(u) = \lambda(\lambda + 1)u + O(u^2).$$

The remainder of the proof of Lemma 2 is presented by Chen and Qi in [3].

CHAPTER FOUR: THE CASE *D* ≥ 1

Lemma 3: *Suppose* $D \geq 1$. *Then* $DA(u) \geq \kappa^2 u$ *for all* $u \in [0,1]$. *Consequently,* $\nexists$ *a traveling wave solution to (2.2) when* $\kappa^2 > DK(n)$, *i.e. when* $v < \sqrt{D / K(n)}$.

Proof: If $D = 1$, then $\alpha + \beta = 1$ from part (*2b*) of Proposition 1. Also we have $u = 1 - \beta$. As well:

$$A(u) = \frac{D\alpha}{v^2} = \frac{\alpha}{v^2} = \kappa^2 u \text{ for all } u \in [0,1].$$

When $D > 1, \quad \forall u \in (0,1)$

$$\begin{aligned}
&P\left[DA - \kappa^2 u\right]' \\
&= P[DA'(u) - \kappa^2] \\
&= D[\kappa^2(P + u) - DA] - P\kappa^2 \\
&= -D[DA - \kappa^2 u] + (D-1)\kappa^2 P \\
&> -D[DA - \kappa^2 u]
\end{aligned}$$

In addition, when *u* is sufficiently small:

$$DA(u) = D(1+\lambda)\lambda u + O(u^2) > [D + \lambda]\lambda u.$$

Substituting $\lambda = \frac{1}{2}\left(\sqrt{4\kappa^2 + D^2} - D\right)$ we have

$$[D + \lambda]\lambda u = \left[D + \frac{1}{2}\left(\sqrt{4\kappa^2 + D^2} - D\right)\right] \left[\frac{1}{2}\left(\sqrt{4\kappa^2 + D^2} - D\right)\right][u].$$

This simplifies to:

$$[D + \lambda]\lambda u = \left[\frac{1}{2}\sqrt{4\kappa^2 + D^2} + \frac{1}{2}D\right] \left[\frac{1}{2}\sqrt{4\kappa^2 + D^2} - \frac{1}{2}D\right][u].$$

Moreover,

$$[D + \lambda]\lambda u = \left[\frac{1}{4}(4\kappa^2 + D^2) - \frac{1}{4}D^2\right]u.$$

Then by Lemma 2:

$$[D+\lambda]\lambda u = \kappa^2 u.$$

Applying the Gronwall's inequality gives $DA > \kappa^2 u$ on (0,1).

■

<u>*Lemma 4:*</u> *Suppose* $D > 1$. *Then,*

$$A(u) < \lambda(1+\lambda)u, \quad P(u) < \lambda u, \quad \forall u \in (0,1)$$

Consequently, ∃ a traveling wave solution to (2.2) when $\lambda(\lambda+1) \leq K(n)$*, i.e. when*

$$v \leq \left[\frac{D}{K(n)}\right]^{\frac{1}{2}} \cdot \left[1 - \left(1 - \frac{1}{D}\right) \cdot \frac{\left(4K(n)+1\right)^{\frac{1}{2}} - 1}{\left(4K(n)+1\right)^{\frac{1}{2}} + 1}\right]^{-\frac{1}{2}}$$

The proof of Lemma 4 is presented by Chen and Qi in [3].

CHAPTER FIVE: THE CASE *D* < 1

<u>*Lemma 5:*</u> *Suppose* $D < 1$. *Then* $A > \kappa^2 u$ *on (0,1). Consequently, when* $\kappa^2 > K(n)$, *i.e.*

$v < \dfrac{D}{\sqrt{K(n)}}$, *there is no traveling wave solution to (2.2).*

<u>*Proof:*</u> From direct calculation

$$P[A-\kappa^2 u]' = PA' - \kappa^2 P = \kappa^2[P+u] - DA - \kappa^2 P = \kappa^2 P + \kappa^2 u - DA - \kappa^2 P = \kappa^2 u - DA.$$

Next add and subtract $\kappa^2 Du$ and so:

$$\kappa^2 u - DA = \kappa^2 u - \kappa^2 Du - DA + D\kappa^2 u = \kappa^2(1-D)u - D(A-\kappa^2 u).$$

Because $D < 1$, from the assumption, then

$$1 - D > 0.$$

Also known is that $\kappa^2 > 0$ and $u > 0$. Moreover, $u \in (0,1)$. Therefore

$$\kappa^2(1-D)u > 0.$$

This gives us the following inequality:

$$\kappa^2(1-D)u - D(A-\kappa^2 u) > -D(A-\kappa^2 u).$$

Now that the following inequality has been established:

$$P[A-\kappa^2 u]' > -D(A-\kappa^2 u).$$

Applying Gronwall's inequality gives

$$A > \kappa^2 u \text{ on } [0,1).$$

It then follows from Lemma 1, that there does not exist any solution to the traveling wave problem.

■

<u>*Lemma 6*</u> *Suppose* $D < 1$. *Then*

$$A(u)(1-u)^{\frac{n}{2}} \le \lambda\left[P(u)+u\right], \quad \forall u \in \left[0,1\right).$$

Proof:

At $u = 0$, the two sides are equal.

Computation in $(0,1]$ shows

$$
\begin{aligned}
&P\Big[(1-u)^{\frac{n}{2}}A - \lambda\big(P+u\big)\Big]' \le 0\\
&= \big(1-u\big)^{\frac{n}{2}}\Big[\kappa^2(P+u) - DA\Big] - \frac{1}{2}nPA\big(1-u\big)^{\frac{n}{2}-1} - \lambda A(1-u)^n\\
&\le -\Big[D + \lambda\big(1-u\big)^{\frac{n}{2}}\Big]\Big[A\big(1-u\big)^{\frac{n}{2}} - \lambda(P+u)\Big] + (P+u)\Big[\big(\kappa^2 - \lambda^2\big)\big(1-u\big)^{\frac{n}{2}} - \lambda D\Big]\\
&= -\Big[D + \lambda\big(1-u\big)^{\frac{n}{2}}\Big]\Big[A\big(1-u\big)^{\frac{n}{2}} - \lambda(P+u)\Big] - \lambda D(P+u)\Big[1 - \big(1-u\big)^{\frac{n}{2}}\Big]\\
&\le -\Big[D + \lambda\big(1-u\big)^{\frac{n}{2}}\Big]\Big[A\big(1-u\big)^{\frac{n}{2}} - \lambda(P+u)\Big]
\end{aligned}
$$

In the first inequality we drop the term

$$-\frac{1}{2}nPA(1-u)^{\frac{n}{2}-1} < 0.$$

In the second inequality the $\kappa^2 - \lambda^2 = \lambda D$.

The proof of Lemma 6 follows from Gronwall's inequality.

■

Proof of Theorem 3: We want to show non-existence of the solution for (2.2). The non-existence follows directly from Lemma 5:

$$\kappa^2 > K(n), \quad \text{when } D < 1.$$

That is, if

$$v < \frac{D}{\sqrt{K(n)}}$$

$\nexists$ a traveling wave solution.

We now prove existence. Simple computation shows that when $v \ge \dfrac{4D}{\sqrt{1+4D}}, \quad \lambda \le \dfrac{1}{4}$. Recall from Lemma 2 that

$$\lambda = \frac{1}{2}\left(\sqrt{4\kappa^2 + D^2} - D\right). \tag{5.1}$$

Also note that if

$$v = \frac{4D}{\sqrt{1 + 4D}}$$

then

$$v^2 = \frac{16D^2}{1 + 4D}.$$

Also recall

$$\kappa = \frac{D}{v}.$$

Thus

$$\frac{D^2}{\kappa^2} = \frac{16D^2}{1 + 4D}$$

and so

$$\kappa^2 = \frac{1 + 4D}{16}.$$

Substituting this value into (5.1), we obtain

$$\lambda = \frac{1}{2}\left(\sqrt{\frac{1 + 4D}{4} + D^2} - D\right)$$

that is

$$\lambda = \frac{1}{2}\left(\frac{1}{2}\sqrt{\left(2D + 1\right)^2} - D\right) = \frac{1}{4}.$$

We now proceed to show that

$$P-\frac{u(1-u)}{2}\leq 0 \text{ on } (0,1).$$

We have

$2P-u(1-u)$

$$\begin{aligned}
&= P(2u-3)+2A(1-u)^n\\
&\leq P(2u-3)+2\lambda\left(P+u\right)(1-u)^{\frac{n}{2}}\\
&= P(2u-3)+2A(1-u)^n \leq 2P\left[u-\frac{3}{2}+\lambda(1-u)^{\frac{n}{2}}\right]-u(1-u)\left[u-\frac{3}{2}+\lambda(1-u)^{\frac{n}{2}}\right]\\
&\quad +u(1-u)\left[2\lambda(1-u)^{\frac{n}{2}-1}+\lambda(1-u)^{\frac{n}{2}}+u-\frac{3}{2}\right]\\
&< \left[u-\frac{3}{2}+\lambda(1-u)^{\frac{n}{2}}\right]\left[2P-u(1-u)\right].
\end{aligned}$$

Since $\lambda\leq\frac{1}{4}\,\forall n\geq 2$, we have

$$2\lambda(1-u)^{\frac{n}{2}-1}+\lambda(1-u)^{\frac{n}{2}}+u-\frac{3}{2}\leq 2\lambda+\lambda(1-u)+u-\frac{3}{2}=2\lambda-\frac{1}{2}+\left(\lambda-1\right)(1-u)\leq 0.$$

Because $2P<u(1+u),\ \forall u\ll 1$, Gronwall's inequality shows that

$$P<\frac{u(1-u)}{2}\ \text{on}\ (0,1).$$

Thus, $P(1) = 0$, which proves existence. ■

CHAPTER SIX: NUMERICAL ANALYSIS SUMMARY

Theoretical results leave a gap in determining the minimum speed, v_{min}. We use numerical analysis to fill-in this gap for v_{min} for various cases of *D* using Matlab®. We tested the robustness of the built-in solvers using the Lotka-Volterra system. The built-in solvers were not up to the task of producing our desired results and thus we chose to test and subsequently implement the explicit fourth-order Runge-Kutta method, as described in Reckenwald [8]. In all cases presented below a small perturbation to the original equation was made.

6.1 The First Order Equation

We start our numerical computation with the first order system. Equation (3.2) is solved for Q' as follows:

$$Q'(u) = -1 + \frac{ku(1-u)^n}{Q(u)} \qquad Q(0) = 0\,. \tag{6.1}$$

Here *D* is 1. The algorithm blows-up or produces incorrect results when diving by $Q(u)$. By making a slight modification, the algorithm reproduced exactly the theoretical results and thus justifies the modification. The modification made is dividing by $Q(u) + 0.001$. For the case of *K*(0), $Q(h) \approx c_1 h$, the result of the numerical analysis is a linear graph (Figure 1). From Lemma 1 we have that *K*(1)=0.25 and *K*(2)=2. Figures 2 and 3 show the numerical results for the traveling wave solution for these two cases. When deviating from the specified *K*(*n*) values, $Q(1)$ is greater than zero. In fact, the greater the departure from the prescribed value, the earlier the traveling wave solution diverges from the anticipated solution.

6.2 Second Order System

The next task is to address the traveling wave solution for (3.6). Solving for $P'(u)$ and $A'(u)$ gives us

$$P'(u) = \frac{\left[A(u)(1-u)^n - P(u)\right]}{P(u)}, \quad \forall u \in \left[0,1\right]$$

$$A'(u) = \frac{\left[\kappa^2(P(u)+u) - DA(u)\right]}{P(u)}, \quad \forall u \in \left[0,1\right]$$

$$P(u) > 0, \quad A(u) > 0, \quad \forall u \in (0,1)$$

$$P(0) = 0, \quad A(0) = 0.$$

(6.2)

Two cases are analyzed: one for small *D* and one for large *D*, where the speed v is varied such that a traveling wave solution exists. Moreover, the minimum speed ($v_{\min}$) is identified.

6.3 Small D

The first value considered is *D* = 0.1. Theorem 1 establishes the range in which the minimum speed occurs. This interval is [0.0707, 0.3381]. For a speed of *v* = 0.34, we first seek to establish a traveling wave solution numerically. Analogous to the first order system explored before, a modification is made to the division by *P(u)* in both equations by adding a small value of 0.001. This modification helps obtain better results, yet *P(1)* ≠ 0. A further adjustment is made by dividing by $P(u) + 0.01$. Once the adjustments are made, consistent and accurate traveling wave solutions are obtained for *v* = 0.34, for various step sizes, i.e. $h = 0.01, 0.005, 0.001$ (Figure 4).

Next we want to find $v_{\min}$ by taking iterative bisections of the interval [0.0707, 0.3381]. The $v_{\min}$ is determined through graphical and tabular numerical analyses. Further fine-tuning of the system is required for consistent results for various step sizes and thus we divide by $P(u) + 0.005.$

The first significant determination done in this work is that v_{min} = 0.135, for D = 0.1.

A similar scenario is conducted for $D = 0.01$ for the interval [0.0071, 0.0392]. Fine-tuning is accomplished by dividing both equations of (6.2) by $P(u) + 0.005$ (Figure 5).

The second significant achievement of this thesis is that v_{min} = 0.0152, for D = 0.01.

6.4 Large D

The first case presented for large *D* is $D = 10$. From Theorem 2, the interval used to investigate the minimum speed for *D* = 10 is $[2.2361, 3.0151]$. Lemma 2 is used to compute the initial values for $P(u)$ and $A(u)$, that is $P(u) = \lambda h$ and $A(u) = \lambda(1+\lambda)h.$ A traveling wave solution is obtained when dividing (6.2) by $P(u) + 0.015$. For a speed of 3.0150 and *n* = 2 a traveling wave solution is established (Figure 6). In a manner similar to the cases of small *D* values, the interval is bisected.

The third, and final significant finding is that v_{min} = 2.923, for D = 10.

Lastly, the case of *D* = 50 is investigated. The interval for associated with the *D* value is $\left[5.0000, 7.0014\right]$. For a speed of 7.0000, *h* = 0.001, a traveling wave solution is established (Figure 7). Because of the large value of *D* the results are not as robust as the other cases for *D*.

CHAPTER SEVEN: RESULTS

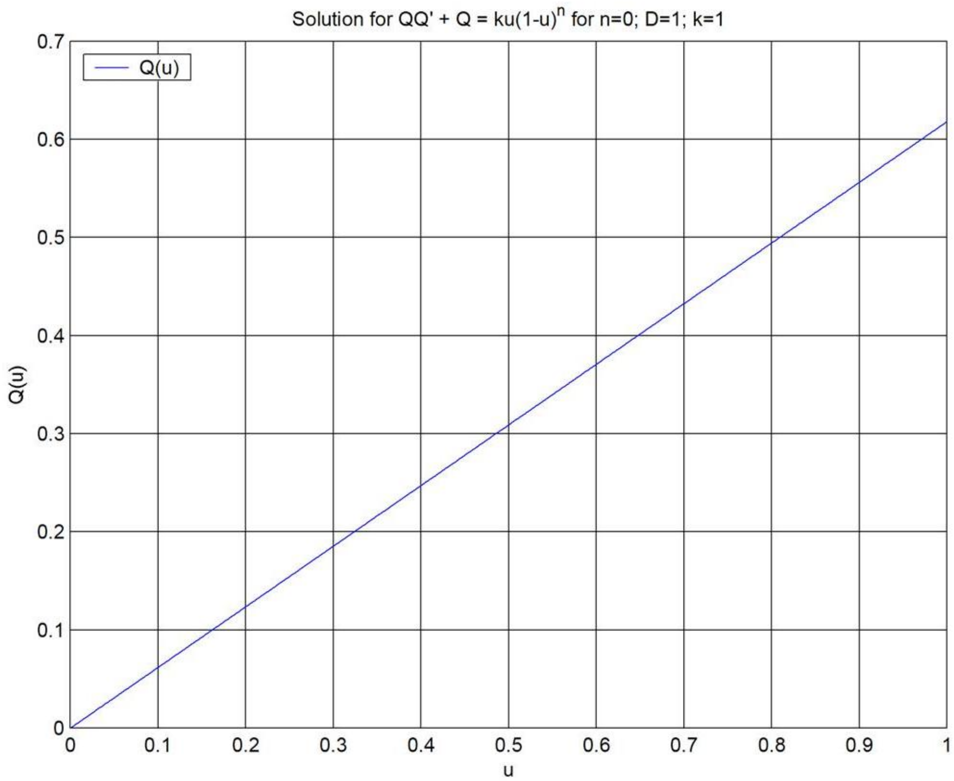

Figure 1

This figure represents the results from the traveling wave equation (6.1) for the case $D = 1$, $n = 0$. As expected, the solution is linear.

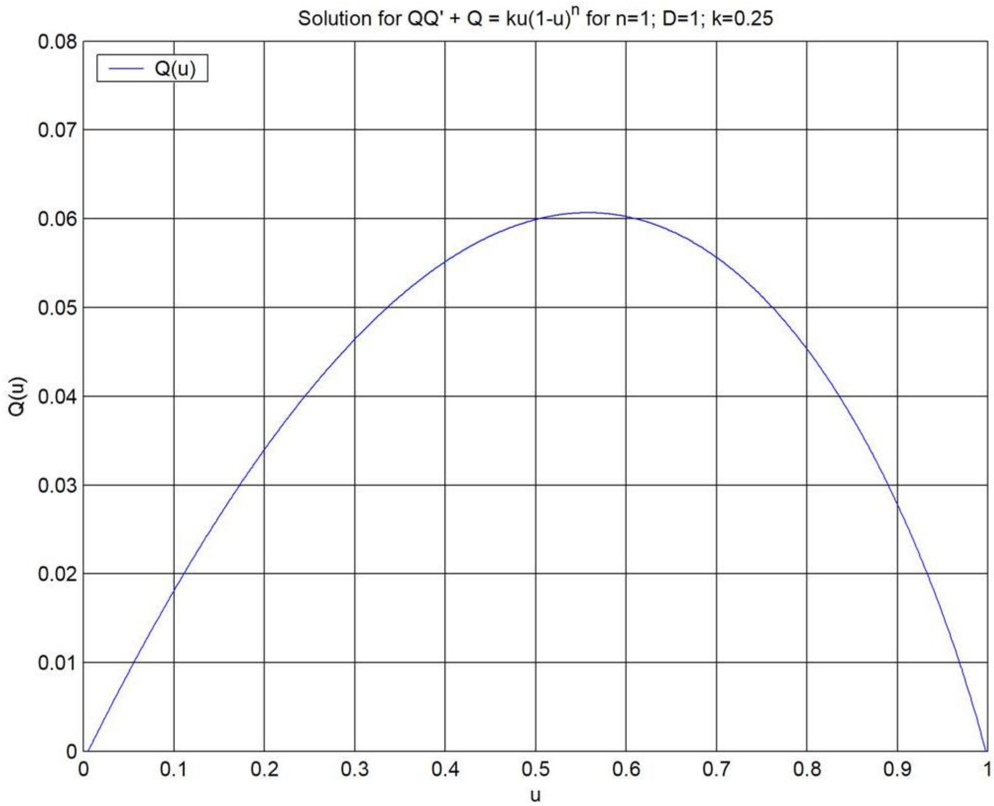

Figure 2

This figure is the results from the traveling wave equation (6.1) for the case $D = 1$, $K(1) = 0.25$.

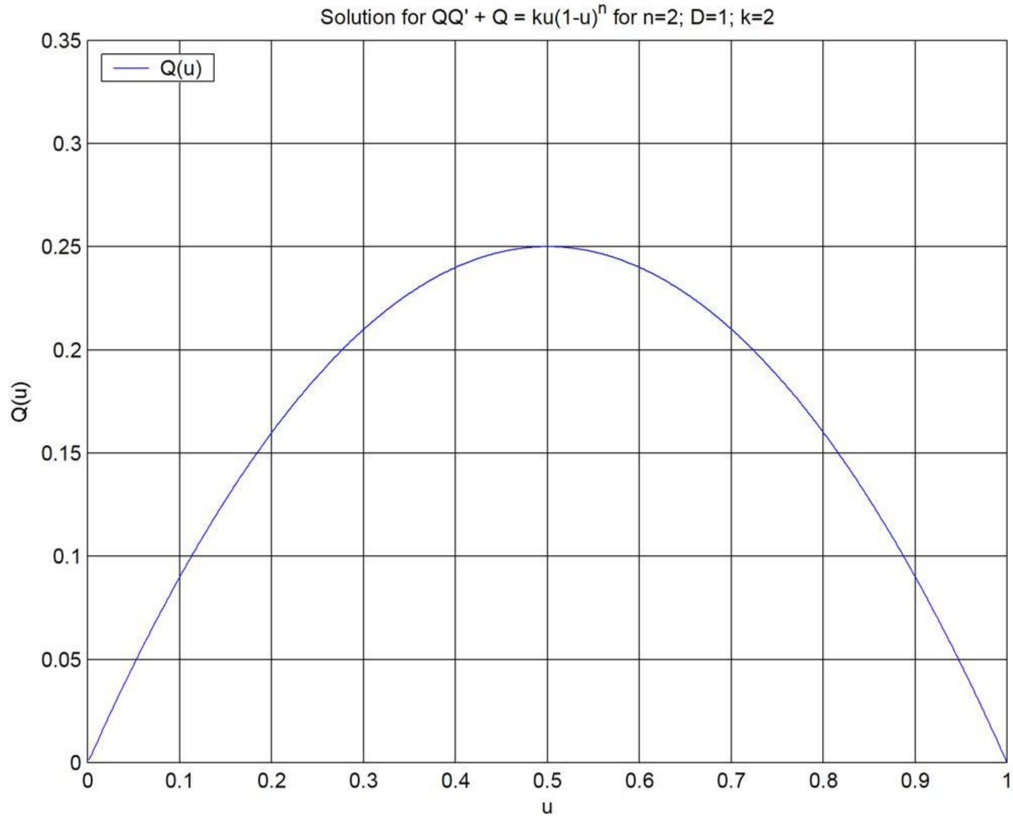

Figure 3

This figure is the results from the traveling wave equation (6.1) for the case $D = 1$, $K(2) = 2$.

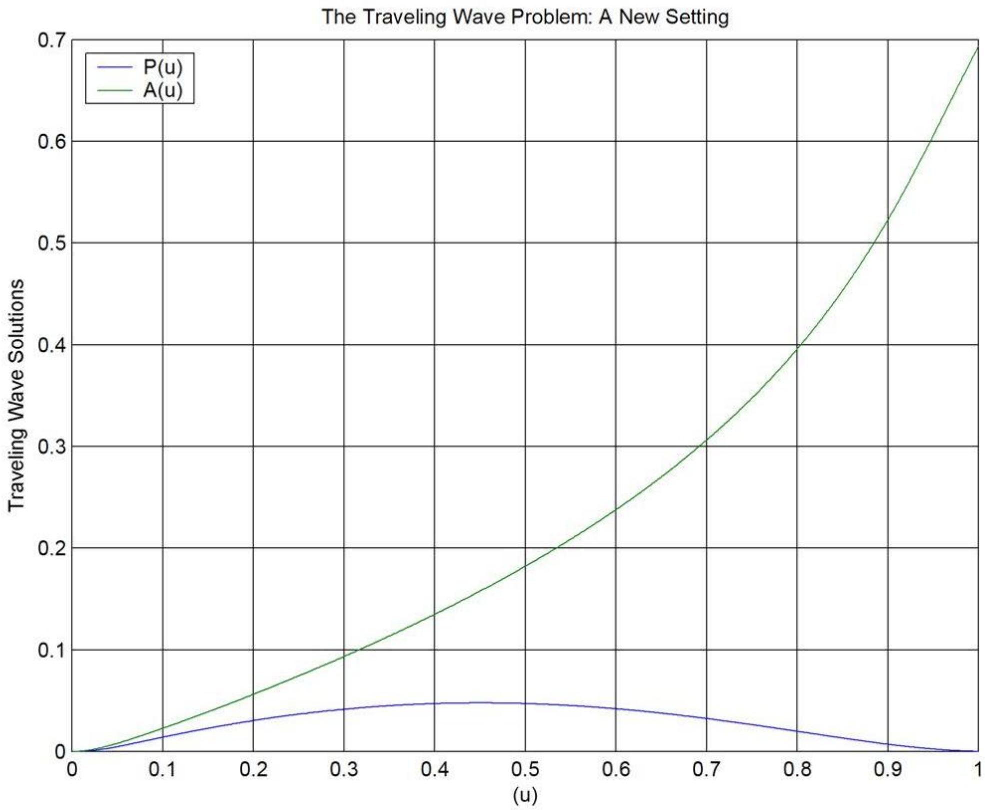

Figure 4

This figure is the results from the traveling wave equation (6.2) for the case $D = 0.1$, $n = 2$, and $v = 0.34$.

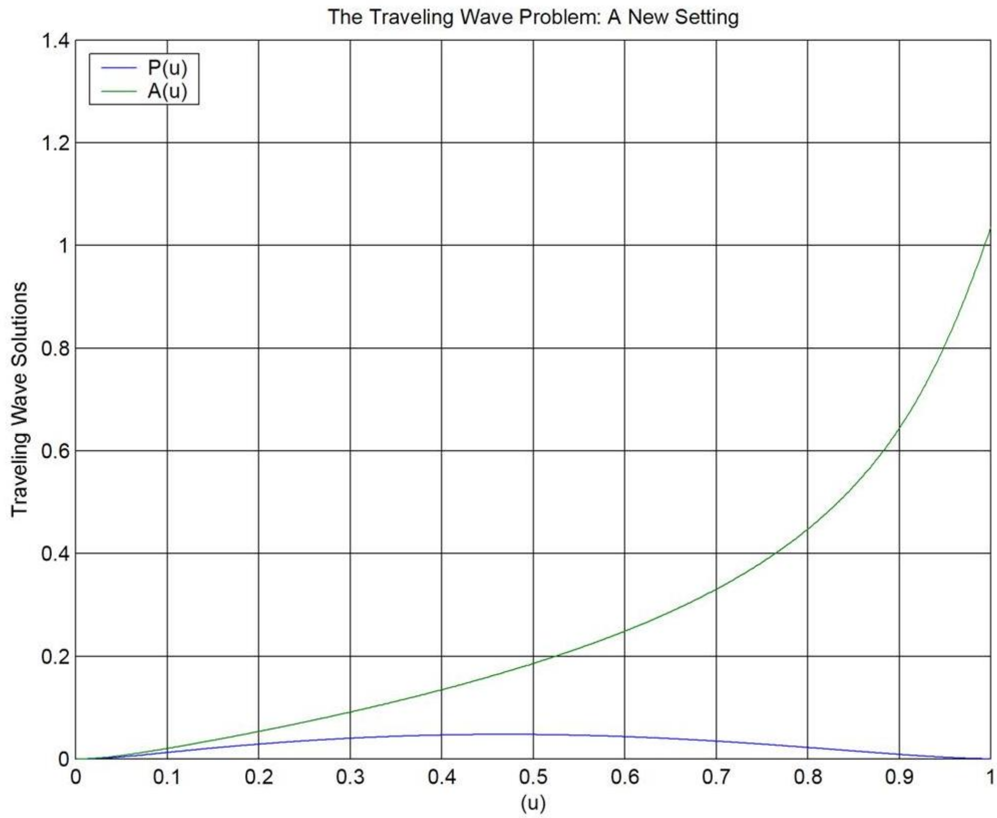

Figure 5

This figure is the results from the traveling wave equation (6.2) for the case $D = 0.01$, $n = 2$, and $v = 0.135$.

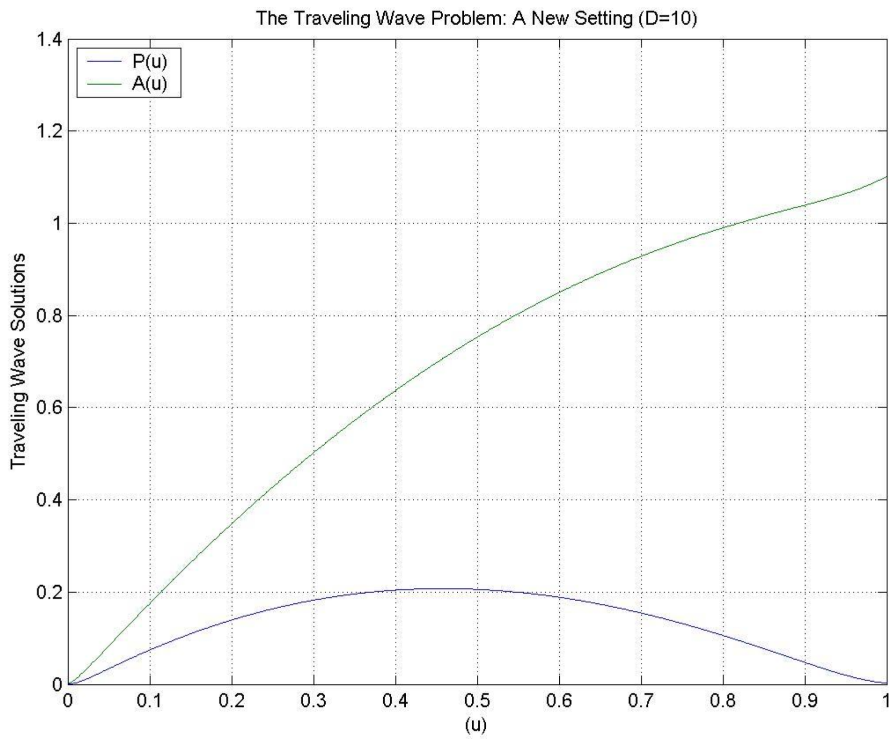

Figure 6

This figure is the results from the traveling wave equation (6.2) for the case $D = 10$, $n = 2$, and $v = 3.0150$.

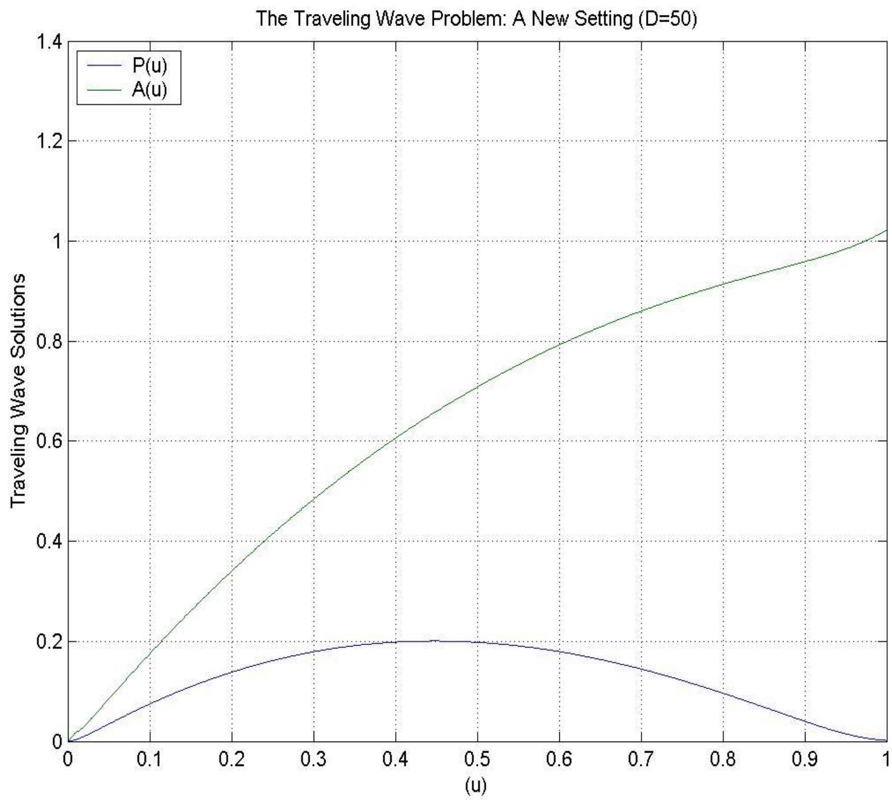

Figure 7

This figure is the results from the traveling wave equation (6.2) for the case $D = 50$, $n = 2$, and $v = 7.0000$.

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