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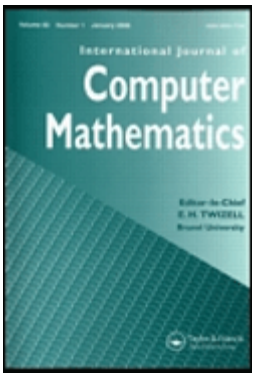

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Singular perturbation analysis for convection-diffusion-reaction equation on nonuniform media (SI - CMMSE - 2006)

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In this paper we study the a one dimensional reaction-diffusion-convection (R-D-C) equation with weak spatial non-uniformities to the diffusion and reaction rates. The convection is represented by a uniform flow field. Singular perturbation analysis will be used to compute the speed of the front as well as the asymptotic solution.

Keywords: Reaction-Diffusion-Convection, Nonuniform Reaction, Nonuniform Diffusion, Singular Perturbation Analysis, Solvability Integral Condition, Propagation of Fronts.

AMS Subject Classifications: 35K57, 46N20, 35B25, 76M45.

1. Introduction

From a physical point of view, the convection-diffusion process and the diffusion-reaction process are fundamental to describe a wide variety of problems in physical, chemical and biological sciences. Nonlinear equations that model such process provide many new insights into the question of interaction of nonlinearity and diffusion. In these problems the propagation of fronts has deserved particular attention of researchers. We can mention, without being exhaust, the works of [1], [2], [3], [6], [7] and [8].

The R-D-C models which have widest range of applicability involve heterogeneities in the diffusion and reaction coefficients. However little work has been developed in this general case. Recently in [10] the authors studied a (R-D) model in a spatially heterogeneous media. They treat separately the case of nonuniform diffusion and nonuniform reaction. In this work while following the procedure in [10] we consider simultaneously heterogeneities in diffusion and reaction.

In this paper we consider weak spatial nonuniformaties to the diffusion and reaction rates. Further, this is a one dimensional study where the convection term is simply to provide a uniform flow.

The paper is organized as follows. In section (2) we present the model. In section (3), we use a singular perturbation analysis and we establish an expression for the asymptotic solution, and the front speed.

2. Problem's formulation

Let consider the reaction-diffusion equation with convection

$$\partial_t \phi = \partial_x [D(\epsilon x)\partial_x \phi] + U(\epsilon x) f(\phi) + \alpha \partial_x \phi \tag{1}$$

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where the function f satisfies $f(0) = f(1) = 0$, and $\phi(x,0) = 1$ for $x < 0$ and $\phi(x,0) = 0$ for $x > 0$. In (1) D and U are, respectively, the dimensionless diffusion coefficient and the reaction rate, ϵ is a small parameter and α is the convection coefficient.

Since we expect solutions to behave like totally developed fronts, we consider a change of independent variables defined **by** $\widehat{x} = \frac{x}{\epsilon}$ **and** $\widehat{t} = \frac{t}{\epsilon}$**. According to these transformations, the derivatives in Eq. (1) can be replaced by**

$$\partial_{\widehat{t}} = \frac{1}{\epsilon}\partial_t, \quad \partial_{\widehat{x}} = \frac{1}{\epsilon}\partial_x, \quad \partial_{\widehat{x}\widehat{x}} = \frac{1}{\epsilon^2}\partial_{xx},$$

where hats denote the new variables. In order to simplify the notation, the hats are dropped for convenience. Then Eq.(1) becomes

$$\epsilon\partial_t\phi = \epsilon^2\partial_x[D(x)\partial_x\phi] + U(x)f(\phi) + \epsilon\alpha\partial_x\phi. \tag{2}$$

In order to have consistency with initial conditions and the existence of a front, we require that the solution ϕ of (1) satisfies $\lim_{x\to-\infty}\phi = 1$ and $\lim_{x\to+\infty}\phi = 0$.

3. Singular Perturbation Analysis

In this section we study equation (2) with

$$U(x) \equiv \beta + \delta\eta_U(x);\ D(x) \equiv 1 + \delta\eta_D(x), \tag{3}$$

where $\delta\eta_U(x)$ and $\delta\eta_D(x)$ are reaction and diffusion perturbations, respectively.

3.1. *General Asymptotic Wavespeed*

This method has been already use in the study of pulled fronts speed. We assume $\delta = O(\epsilon)$, i.e., $\delta \equiv \sigma\epsilon$, where $\sigma = O(1)$.

Eqs. (2) and (3), together with the corresponding boundary conditions, becomes

$$\epsilon\partial_t\phi = \epsilon^2\partial_x[(1 + \delta\eta_D(x))\partial_x\phi] + (\beta + \delta\eta_U(x))f(\phi) + \epsilon\alpha\partial_x\phi \tag{4}$$

$$\lim_{x\to-\infty}\phi = 1, \ \lim_{x\to+\infty}\phi = 0.$$

In order to study **Eq.** (4) we will make a nonrigorous asymptotic analysis. We assume that the domain is divided into **three regions** according to the space scales: a boundary layer region, whose width is $O(\epsilon)$, in which ϕ is rapidly varying; and **two external regions** in which ϕ is almost constant, i.e., either $\phi = O(\epsilon^{n_1})$ or $\phi = 1 + O(\epsilon^{n_2})$, $n_1, n_2 \in \mathbb{R}^+$.

In order to solve Eq. (4) in the outer regions we expand ϕ as follows

$$\phi(x,t;\epsilon) = \phi_0(x,t) + \epsilon\phi_1(x,t) + \epsilon^2\phi_2(x,t) + O(\epsilon^3).$$

and consequently

$$f(\phi) = f(\phi_0) + f^{(1)}(\phi_0)\phi_1\epsilon + \frac{1}{2}f^{(2)}(\phi_0)\phi_1^2\epsilon^2 + f^{(1)}(\phi_0)\phi_2\epsilon^2 + ...,$$

where $f^{(1)}(\phi_0) = \frac{df(\phi)}{d\phi}|_{\phi=\phi_0}$ and $f^{(2)}(\phi_0) = \frac{d^2f(\phi)}{d\phi^2}|_{\phi=\phi_0}$.

By substituting the previous equation into Eq. (4) and collecting terms with the same powers of ϵ we get

$$\beta f(\phi_0) = 0, \quad \lim_{x\to-\infty} \phi_0 = 1, \quad \lim_{x\to\infty} \phi_0 = 0 \tag{5}$$

$$\partial_t \phi_0 = \beta f^{(1)}(\phi_0)\phi_1 + \sigma\eta_U(x) f(\phi_0) + \alpha\partial_x\phi_0, \quad \lim_{x\to\pm\infty} \phi_1 = 0 \tag{6}$$

and

$$\partial_t \phi_1 = \partial_{xx}\phi_0 + \beta\frac{1}{2} f^{(2)}(\phi_0)\phi_1^2 + \sigma\eta_U(x) f^{(1)}(\phi_0)\phi_1 + \beta f^{(1)}(\phi_0)\phi_2 + \alpha\partial_x\phi_1, \quad \lim_{x\to\pm\infty} \phi_2 = 0. \tag{7}$$

The solution of Eq. (5) is $\phi_0 = 1$ in the left of the boundary layer and $\phi_0 = 0$ in the right of the boundary layer. The solutions of Eqs. (6) and (7) are $\phi_1 \equiv 0$ and $\phi_2 \equiv 0$, respectively. Thus, $\phi(x,t;\epsilon) = O(\epsilon^3)$ in the right of the boundary layer and $\phi(x,t;\epsilon) = 1 + O(\epsilon^3)$ in the left of the boundary layer. **As we can see, for this order of magnitude, there is no difference in the shape of the front.**

In order to study the dynamics in the interior of the boundary layer, we translate Eq. (4) to the reference frame of the front, i.e.,**we define the new variable** $z\epsilon = x - S(t)$ where $S(t)$ represents the position of the front.

The derivatives in **Eq.** (4) are transformed according to

$$\partial_t \to -\frac{\dot{S}}{\epsilon}\partial_z + \partial_t, \quad \partial_{xx} \to \frac{1}{\epsilon^2}\partial_{zz}, \quad \partial_x \to \frac{1}{\epsilon}\partial_z, \tag{8}$$

where $\dot{S} = \frac{dS}{dt}$.

Taking into account [10], we expand ϕ and S in powers of ϵ we have

$$\phi(z,t) = \phi_0(z) + \epsilon\phi_1(z,t) + \epsilon^2\phi_2(z,t) + ... \tag{9}$$

$$S(t) = S_0(t) + \epsilon S_1(t) + \epsilon^2 S_2(t) + ...$$

and, consequently,

$$\eta_U(x) = \eta_U(S_0 + z\epsilon + S_1\epsilon + ...) \simeq \eta_U(S_0) + \eta_U'(S_0)(z + S_1)\epsilon + ... \tag{10}$$

$$\eta_D(x) = \eta_D(S_0 + z\epsilon + S_1\epsilon + ...) \simeq \eta_D(S_0) + \eta_D'(S_0)(z + S_1)\epsilon + ... \tag{11}$$

$$f(\phi) = f(\phi_0) + f^{(1)}(\phi_0)\phi_1\epsilon + \frac{1}{2} f^{(2)}(\phi_0)\phi_1^2\epsilon^2 + f^{(1)}(\phi_0)\phi_2\epsilon^2 + ..., \tag{12}$$

where $\eta_U'(S_0) = \dfrac{d\eta_U(x)}{dx}|_{x=S_0}$, $\eta_D'(S_0) = \dfrac{d\eta_D(x)}{dx}|_{x=S_0}$.

Inserting Eqs. (8), (9), (10), (11) and (12) into (4)
and after some calculations, we get the $O(1)$ equation

$$\partial_{zz}\phi_0 + (\dot{S}_0 + \alpha)\partial_z\phi_0 + \beta f(\phi_0) = 0. \tag{13}$$

The $O(\epsilon)$ terms are given by

$$\partial_{zz}\phi_1 + (\dot{S}_0 + \alpha)\partial_z\phi_1 + \beta f^{(1)}(\phi_0)\phi_1 = -\dot{S}_1\partial_z\phi_0 - \sigma\eta_U(S_0)f(\phi_0) - \sigma\eta_D(S_0)\partial_{zz}\phi_0.$$

Introducing the operator

$$\mathcal{L} = \partial_{zz} + (\dot{S}_0 + \alpha)\partial_z + \beta f^{(1)}(\phi_0)$$

the $O(\epsilon)$ equation is equivalent to

$$\mathcal{L}(\phi_1) = -\dot{S}_1\partial_z\phi_0 - \sigma\eta_U(S_0)f(\phi_0) - \sigma\eta_D(S_0)\partial_{zz}\phi_0. \tag{14}$$

Finally, we get the terms in $O(\epsilon^2)$

$$\begin{aligned}\partial_{zz}\phi_2 + (\dot{S}_0 + \alpha)\partial_z\phi_2 + \beta f^{(1)}(\phi_0)\phi_2 = &-\dot{S}_1\partial_z\phi_1 - \beta\frac{1}{2}f^{(2)}(\phi_0)\phi_1^2 + \partial_t\phi_1 - \dot{S}_2\partial_z\phi_0 \\ &-\sigma\eta_U(S_0)f^{(1)}(\phi_0)\phi_1 - \sigma\eta'_U(S_0)(z+S_1)f(\phi_0) \\ &-\sigma\eta_D(S_0)\partial_{zz}\phi_1 - \sigma\eta'_D(S_0)\partial_z\phi_0 \\ &-\sigma\eta'_D(S_0)(z+S_1)\partial_{zz}\phi_0.\end{aligned}$$

Since $\phi_0 = \phi_0(z)$, Eq. (13) is equivalent to the homogeneous parabolic reaction-diffusion equation translated to the front reference frame, $z = x - ct$. The front travels at constant speed c, with $c = \alpha + \dot{S}_0$. Integrating the above equation with respect to t we get $S_0 = (c-\alpha)t$, where we assumed $S(0) = 0$.

The solvability integral condition of Eq. (14) is $\int_{-\infty}^{+\infty}\psi\mathcal{L}(\phi_1)dz = 0$ [9], where ψ is such that $\mathcal{L}^\dagger(\psi) = 0$, $\mathcal{L}^\dagger = \partial_{zz} - (\dot{S}_0 + \alpha)\partial_z + \beta f^{(1)}(\phi_0)$ being $\mathcal{L}^\dagger$ the self-adjoint operator. It is easy to show that $\psi = e^{cz}\frac{d\phi_0}{dz}$ is an eigen-function of $\mathcal{L}^\dagger$ with null eigenvalue.

Therefore, the solvability integral (14) may be rewritten

$$\int_{-\infty}^{+\infty} e^{cz}\frac{d\phi_0}{dz}\left[-\dot{S}_1\partial_z\phi_0(z) - \sigma\eta_U(S_0)f(\phi_0) - \sigma\eta_D(S_0)\partial_{zz}\phi_0\right] = 0 \tag{15}$$

Using (13), we get

$$\int_{-\infty}^{+\infty} e^{cz}\frac{d\phi_0}{dz}[-\dot{S}_1\partial_z\phi_0 - \sigma\eta_U(S_0)f(\phi_0) + \sigma\eta_D(S_0)(\dot{S}_0+\alpha)\partial_z\phi_0 + \beta\sigma\eta_D(S_0)f(\phi_0)] = 0 \tag{16}$$

and therefore

$$\dot{S}_1 = -\frac{\sigma(\eta_U(S_0) - \beta\eta_D(S_0))\int_{-\infty}^{+\infty} e^{cz}\frac{d\phi_0}{dz}f(\phi_0)dz - (\dot{S}_0+\alpha)\sigma\eta_D(S_0)\int_{-\infty}^{+\infty} e^{cz}(\frac{d\phi_0}{dz})^2dz}{\int_{-\infty}^{+\infty} e^{cz}(\frac{d\phi_0}{dz})^2dz},$$

with $c = \dot{S}_0 + \alpha$.

Attending to the equation (13), that can be expressed as

$$\beta f(\phi_0) = -\partial_{zz}\phi_0 - (\dot{S}_0+\alpha)\partial_z\phi_0, \quad c = \alpha + \dot{S}_0$$

and using integrating by parts, the integral $\int_{-\infty}^{+\infty} e^{cz}\frac{d\phi_0}{dz}\beta f(\phi_0)dz$ that appears in the numerator

of $\dot{S}_1$ can be simplified as follows

$$\int_{-\infty}^{+\infty} e^{cz}\frac{d\phi_0}{dz}\beta f(\phi_0)dz = -\int_{-\infty}^{+\infty} e^{cz}\frac{d\phi_0}{dz}\frac{d^2\phi_0}{dz^2}dz$$
$$-c\int_{-\infty}^{+\infty} e^{cz}(\frac{d\phi_0}{dz})^2dz$$
$$= -\frac{1}{2}c\int_{-\infty}^{+\infty} e^{cz}(\frac{d\phi_0}{dz})^2dz.$$

Then, we have the following simplification of $\dot{S}_1$

$$\dot{\mathbf{S}}_\mathbf{1} = \frac{\mathbf{c}\sigma}{\mathbf{2}\beta}(\eta_\mathbf{U}(\mathbf{S_0}) + \beta\eta_\mathbf{D}(\mathbf{S_0})).$$

Taking into account $\dot{S}_0$ and $\dot{S}_1$ and after inverting the hyperbolic scaling, $v(t)$ **has the following simplification**

$$\mathbf{v(t)} \simeq (\mathbf{c}-\alpha) + \frac{\mathbf{c}\delta}{\mathbf{2}\beta}[\eta_\mathbf{U}((\mathbf{c}-\alpha)\mathbf{t}\epsilon) + \beta\eta_\mathbf{D}((\mathbf{c}-\alpha)\mathbf{t}\epsilon)] + \mathbf{O}(\delta^\mathbf{2}).$$

3.2. *General Asymptotic Solution*

In this section we will construct an approximation for the solution of Eqs. (2) and (3). We begin by solving Eq.(14).

Initially we prove that $\mathcal{L}(d\phi_0/dz) = 0$ and use this fact to construct a solution for Eq. (14) **of** the form $\phi_1(z,t) = (d\phi_0/dz) + (d\phi_0/dz)zF(t)$, where $F(t)$ is obtained from Eq. (14) and $\mathcal{L}(d\phi_0/dz) = 0$. **In fact**

$$\begin{aligned}\mathcal{L}\left(\frac{d\phi_0}{dz}\right) &= \partial_{zz}\left(\frac{d\phi_0}{dz}\right) + (\dot{S}_0+\alpha)\partial_z\left(\frac{d\phi_0}{dz}\right) + \beta f^{(1)}(\phi_0)\left(\frac{d\phi_0}{dz}\right)\\ &= \partial_{zzz}(\phi_0) + (\dot{S}_0+\alpha)\partial_{zz}(\phi_0) + \partial_z(\beta f(\phi_0))\\ &= \partial_z(\partial_{zz}\phi_0 + (\dot{S}_0+\alpha)\partial_z\phi_0 + \beta f(\phi_0))\\ &= 0,\end{aligned}$$

because $\partial_{zz}\phi_0 + (\dot{S}_0+\alpha)\partial_z\phi_0 + \beta f(\phi_0) = 0$.

On the other hand we have that

$$\begin{aligned}\mathcal{L}(\phi_1) &= \mathcal{L}\left(\left(\frac{d\phi_0}{dz}\right) + \left(\frac{d\phi_0}{dz}\right)zF(t)\right)\\ &= -(\dot{S}_0+\alpha)\left(\frac{d\phi_0}{dz}\right)F(t) - 2\beta f(\phi_0)F(t). \qquad (17)\end{aligned}$$

We observe that in the establishment of (17) we used

$$\left(\frac{d^3\phi_0}{dz^3}\right) + (\dot{S}_0+\alpha)\left(\frac{d^2\phi_0}{dz^2}\right) + \beta f^{(1)}(\phi_0)\left(\frac{d\phi_0}{dz}\right) = \mathcal{L}\left(\frac{d\phi_0}{dz}\right) = 0$$

and

$$\left(\frac{d^2\phi_0}{dz^2}\right) = -(\dot{S}_0 + \alpha)\left(\frac{d\phi_0}{dz}\right) - \beta f(\phi_0).$$

Attending to Eq. (13), Eq. (14) may be rewritten as

$$\mathcal{L}(\phi_1) = [-\dot{S}_1 + \sigma\eta_D(S_0)(\dot{S}_0 + \alpha)]\partial_z\phi_0 + [-\sigma\eta_U(S_0) + \beta\sigma\eta_D(S_0)]f(\phi_0) \tag{18}$$

and according to the equivalence between equations (17) and (18) , we get

$$-(\dot{S}_0 + \alpha)\left(\frac{d\phi_0}{dz}\right)F(t) - 2\beta f(\phi_0)F(t) = [-\dot{S}_1 + \sigma\eta_D(S_0)(\dot{S}_0 + \alpha)]\partial_z\phi_0 + [-\sigma\eta_U(S_0) + \beta\sigma\eta_D(S_0)]f(\phi_0). \tag{19}$$

Inserting $\dot{S}_1 = \frac{1}{2\beta}c\sigma[\eta_U(S_0) - \beta\eta_D(S_0)] + c\sigma\eta_D(S_0)$, with $c = \dot{S}_0 + \alpha$, into Eq. (19), it can be easily checked that

$$F(t) = \frac{1}{2\beta}\sigma[\eta_U(S_0) - \beta\eta_D(S_0)]. \tag{20}$$

and therefore

$$\phi_1(z,t) = \frac{d\phi_0}{dz}\left[1 + \frac{1}{2\beta}\sigma\left[\eta_U((c-\alpha)t) - \beta\eta_D((c-\alpha)t)\right]z\right]. \tag{21}$$

3.3. *Specific Asymptotic Solutions*

In this section we will present a specific asymptotic solution.

Observe that, for the reaction terms of the form $f(\phi) = \phi^{q+1}(1-\phi^q)$, $q \geq 1$, the exact solutions, ϕ_0, of the equation (13) are well now in literature (see [6], [10]). In this case ϕ_0 takes the form

$$\phi_0(z) = \frac{1}{(1+\exp(dz))^a}, \quad c = \frac{\sqrt{\beta}}{\sqrt{1+q}}, \quad d = qc, \quad a = \frac{1}{q}. \tag{22}$$

Let us assume $\sigma = 1$, $\alpha = 0$ in the Eq.(4) and $q = 1$ in (22).Taking into account that

$$z\epsilon + S(t) = x,$$

the asymptotic solution is represented by

$$\phi(x,t) = \phi_0(x) + \epsilon\phi_1(x,t),$$

where

$$\phi_0(x,t) = \frac{1}{1+\exp\left[\frac{\sqrt{\beta}}{\sqrt{2\epsilon}}(x - S(t))\right]}$$

and

$$\phi_1(x,t) = -\frac{c\exp\left[c\left(\frac{x-S(t)}{\epsilon}\right)\right]}{\left[1+\exp\left[c\left(\frac{x-S(t)}{\epsilon}\right)\right]\right]^2}\left[1+\frac{1}{2\beta}\sigma\left(\eta_U-\beta\eta_D\right)\frac{x-S(t)}{\epsilon}\right].$$

4. Illustration of the Solution Profiles

In this section, we consider a uniform mesh with uniform time steps and we will illustrate the asymptotic solution profiles at various time.

Let us consider the following expressions for the diffusion

$$D(x) = \epsilon\eta_{D(x)} + 1,$$
$$\eta_{D(x)} = 0.4 - [(x/0.9)+1]^3\exp[(0.9)^4 - (x+0.9)^4]$$

and the reaction

$$U(x) = \epsilon\eta_{U(x)} + \beta,$$
$$\eta_{U(x)} = [(x/0.8)+1]^3\exp[(0.8)^4 - (x+0.8)^4], \beta \in \mathbb{R}^+.$$

The following graphics show the diffusion and the reaction for $\beta = 1$.

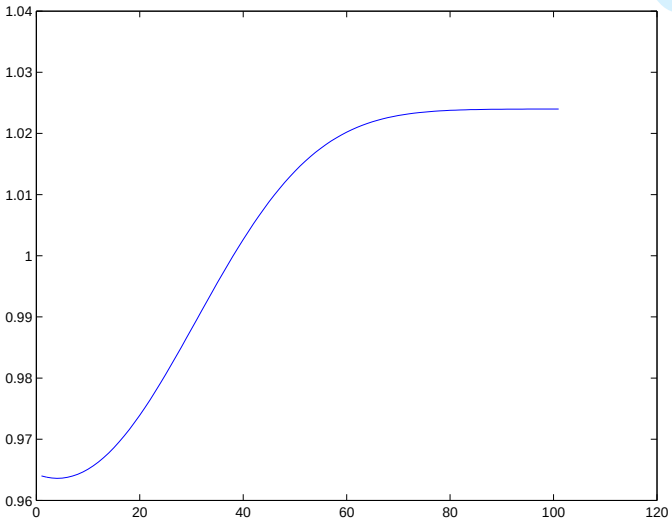

Figure 1. Diffusion

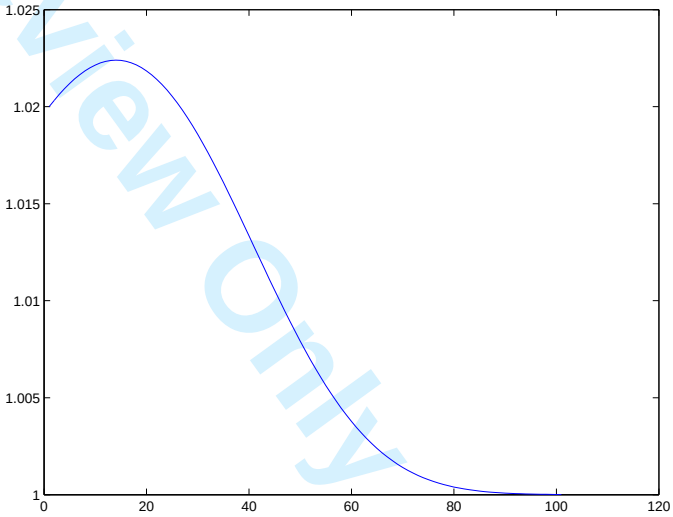

Figure 2. Reaction, $\beta = 1$

For this specific diffusion and reaction, we will present the asymptotic solution profiles at various times.

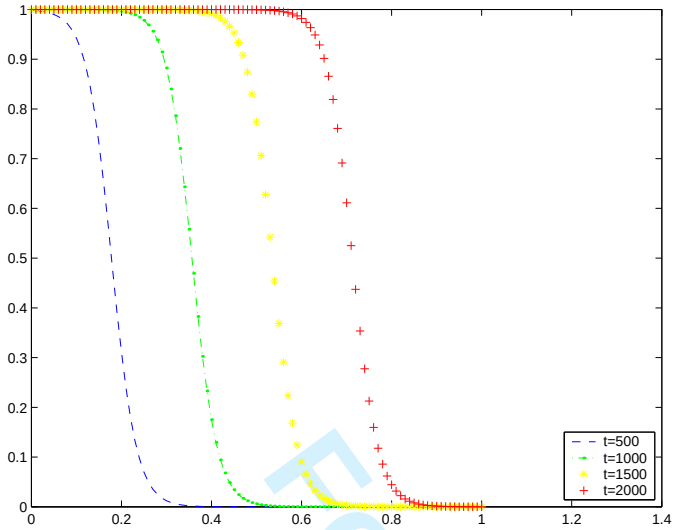

Figure 3. Asymptotic solutions for $\epsilon = 0.02$ and different values of t.

We conclude that, the solution behaves like a traveling wave.

Then, we illustrate the effect of the spatial uniform and non-uniform reaction and diffusion on the asymptotic solution at a specific time, as we can see in the next graphs.

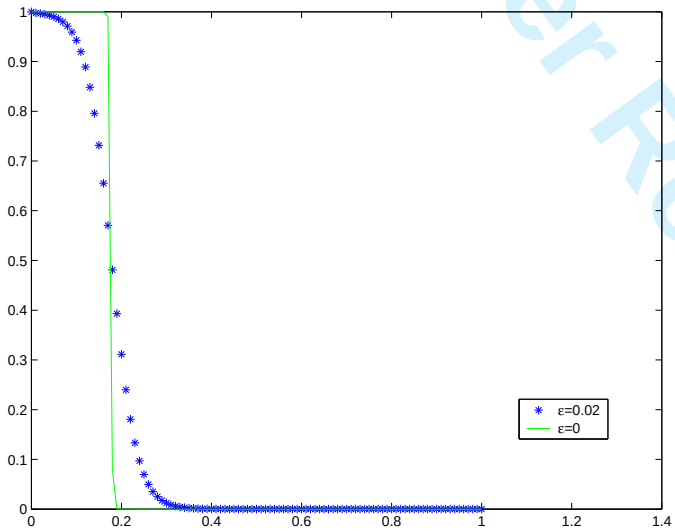

Figure 4. Asymptotic solutions for $t = 500$ and different values of ϵ

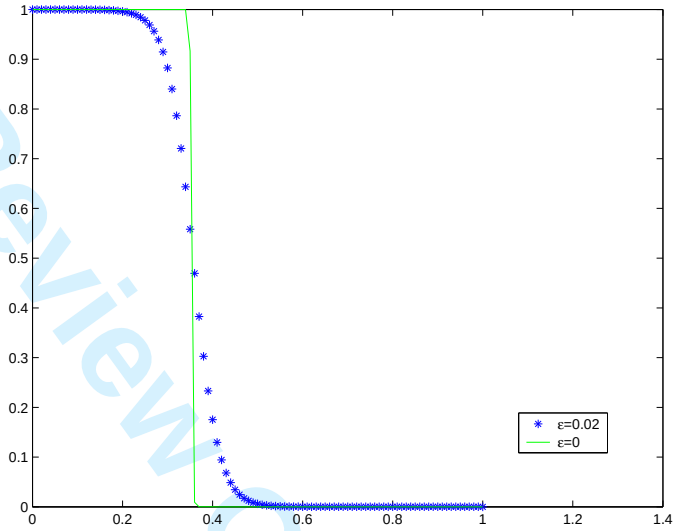

Figure 5. Asymptotic solutions for $t = 1000$ and different values of ϵ

Let us remark that,we obtained other numerical results that will not go to be illustrated, where we concluded that, for small values of ϵ there is a good agreement between the "exact solution"- which is in fact a numerical solution computed in a refined mesh - and the asymptotic solution.

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4.1. *References*

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