THE FOURTH ORDER DIFFUSION MODEL FOR A BI-FLUX MASS TRANSFER

Maosheng Jiang

Tese de Doutorado apresentada ao Programa de Pós-graduação em Engenharia Civil, COPPE, da Universidade Federal do Rio de Janeiro, como parte dos requisitos necessários à obtenção do título de Doutor em Engenharia Civil.

Orientador: Luiz Bevilacqua

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灯不拨不亮，理不辩不明

An oil lamp becomes brighter after trimming, a truth becomes clearer after being discussed.

当局者迷, 旁观者清

The spectators see more of the game than the players.

一图抵万言

A picture is worth a thousand words.

This thesis is dedicated to my loving parents,
Xiufang Jiang and Xiaoying Liu,
my sister Yujuan Jiang
and my wife, Delan Duan,
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.

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O MODELO DE DIFUSÃO DE QUARTA ORDEM PARA UMA TRANSFERÊNCIA DE MASSA BI-FLUXO

Maosheng Jiang

Março/2017

Orientador: Luiz Bevilacqua

Programa: Engenharia Civil

A abordagem discreta é empregada para a difusão com retenção para obter a equação de quarta ordem, o que sugere a introdução de um segundo fluxo levando à associação da teoria bi-fluxo com novos parâmetros: fração β e coeficiente de reatividade R. O objetivo desta tese é explorar a Embora comparando o comportamento da concentração e os dois fluxos com o modelo clássico, principalmente pelo método de elementos finitos de Galerkin. Mostra-se que o processo pode ser acelerado ou retardado dependendo da relação entre R e β, para o meio isotrópico. Dependendo da definição do segundo fluxo em função desses parâmetros e da relação $\beta = \beta(R)$, o comportamento inesperado aumentando a concentração logo após a introdução de um impulso inicial que se opõe à tendência natural de dispersão, pode se desenvolver em uma recuperação restrita. O coeficiente de reatividade R considerado como um atrator variando no espaço e no tempo de acordo com uma lei de difusão é proposto para simular caixa de nutrientes atraindo partículas biológicas. Finalmente, são apresentados dois casos típicos de difusão não-linear que representam dinâmicas de reações químicas. O modelo bi-fluxo tende a regularizar as soluções.

Abstract of Thesis presented to COPPE/UFRJ as a partial fulfillment of the requirements for the degree of Doctor of Science (D.Sc.)

THE FOURTH ORDER DIFFUSION MODEL FOR A BI-FLUX MASS TRANSFER

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Department: Civil Engineering

The discrete approach is employed for diffusion with retention to obtain the fourth order equation, which suggests the introduction of second flux leading to bi-flux theory association with new parameters: fraction β and reactivity coefficient R. The purpose of this thesis is to explore the bi-flux theory though comparing the behavior of concentration and the two fluxes with the classical model mainly by Galerkin finite element method. It is shown that the process may be accelerated or delayed depending on the relation between R and β, for isotropic medium. Depending on the definition of the second flux as function of these parameters and the relation $\beta = \beta(R)$, unexpected behavior increasing the concentration just after the introduction of an initial pulse opposing the natural tendency to disperse, can develop on a restricted regains. Reactivity coefficient R considered as an attractor varying in space and time according to a diffusion law is proposed to simulate nutrient box attracting biological particles. Finally two typical cases of non-linear diffusion representing dynamics of chemical reactions are presented. The bi-flux model tends to regularize the solutions.

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Chapter 1

Introduction

The initial motivation leading to the diffusion approach presented here was a population dynamics problem firstly reported by the LNCC group working in applied mathematics and computational modeling. The motivation was the analysis of population dynamics and its impact on ecological questions (Simas, 2012). For sake of completeness we will present in this section the main steps leading to diffusion with retention for one-dimensional space R^1.

An important problem for the rivers in the Amazon region is the invasion by exotic species that tends to disrupt the ecological equilibrium of the region. That is, we may think of a given population marching to occupy a certain territory. To make the model more realistic consider two clusters of individuals composing the invading group. The warriors whose mission is to fight to conquer new areas and a second group consisting of individuals in charge of settle down. Therefore we may think of two different groups moving with different speeds as shown in Fig.1.1.

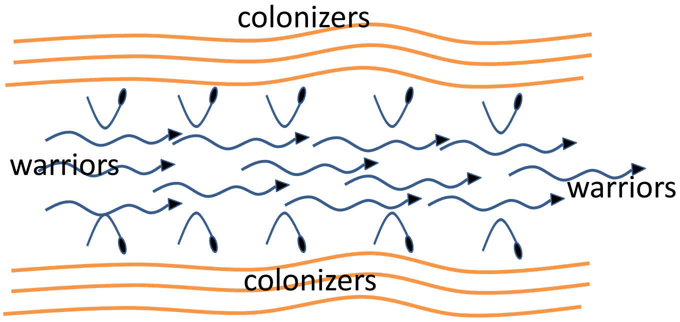
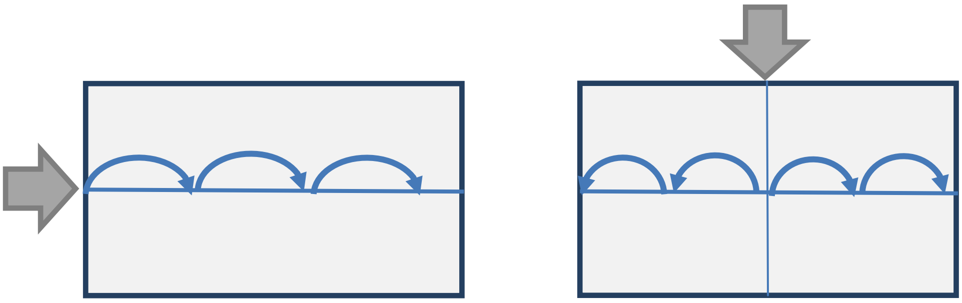


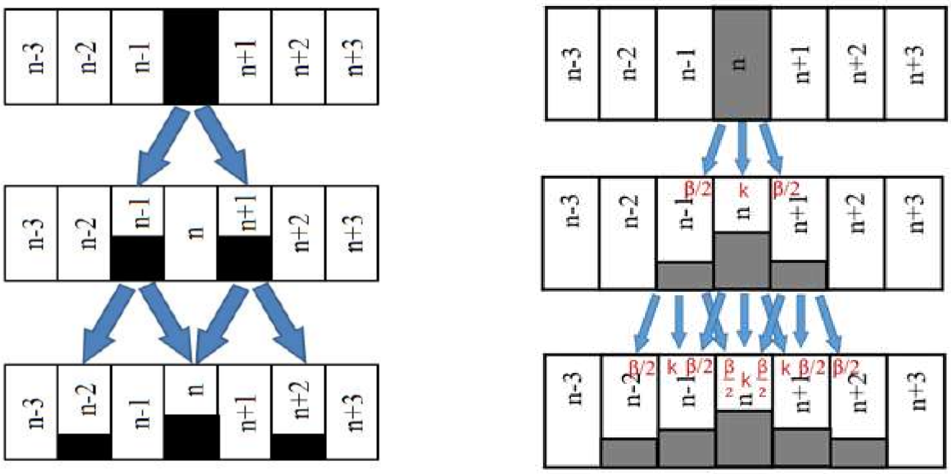
Fig.1.1. Invading population occupying a given field

In order to model this type of behavior it was used a discrete approach. Assume the scattering process consisting of an invading population with the purpose to settle down. It is possible to consider at least two ways to model the invasion strategy. If the invasion progress along a corridor in just one direction the process is equivalent to a wave front. If, however, the invading population find a weak point in the middle of the native population the invasion can be modelled like a diffusion process. This case may happen in cases of tumors spreading in a living organism. Fig. 1.2 displays these two invading processes.



(a) (b)

Fig.1.2. Two possible invasion procedures. (a) wave front, (b) spreading from a given point



(a) (b)

Fig.1.3. Evolution of the diffusing process. (a) without retention, (b) with partial retention. The fraction k of the contents is retained while the complement (1-k) is equally distributed to the right and left cells, β=1-k.

The different processes of mass transport considering retention was discussed in (Bevilacqua L., *etal.*,2011a). Retention introduced in the process intended to take into account the colonizers moving slowly to settle down on the new territory makes the main difference in the analytical expression for the wave and diffusion problems.

For sake of introduction let us examine the evolution of the mass transfer with a discrete approach. Figure 1.3 shows the mass distribution in a given time for a cell chain, without retention (a) and with partial retention (b). For the case indicated in Fig.1.3(a) there is no retention and all the contents contained in a cell n is equally distribute to the left and to the right. We are assuming for all cases symmetric distribution

Consider the classical problem free of retention Fig.1.3-a. The mass distribution for cells n-1, n, n+1 for time t-1 an t is clearly given in the expressions (1.1-a) and (1.1-b).

$$q_n^t = \frac{1}{2} q_{n-1}^{t-1} + \frac{1}{2} q_{n+1}^{t-1} \tag{1.1-a}$$

$$q_n^{t+1} = \frac{1}{2} q_{n-1}^{t} + \frac{1}{2} q_{n+1}^{t} \tag{1.1-b}$$

Consider the difference:

$$q_n^{t+1} - q_n^t = \frac{1}{2} q_{n-1}^{t} + \frac{1}{2} q_{n+1}^{t} - \left(\frac{1}{2} q_{n-1}^{t-1} + \frac{1}{2} q_{n+1}^{t-1} \right)$$

The right hand side written for the time $t-1$ and rearranging the terms gives:

$$q_n^{t+1} - q_n^t = \frac{1}{4}\left(q_{n-2}^{t-1} - 2q_{n-1}^{t-1} + q_n^{t-1}\right) + \frac{1}{4}\left(q_n^{t-1} - 2q_{n+1}^{t-1} + q_{n+2}^{t-1}\right)$$

Recalling that $\Delta^2 f_k = f_{k-1} - 2f_k + f_{k+1}$, the above equation reads:

$$q_n^{t+1} - q_n^t = \frac{1}{4}\left(\Delta^2 q_{n-1}^{t-1} + \Delta^2 q_{n+1}^{t-1}\right)$$

Recalling the difference $q_n^{t+1} - q_n^t = \Delta q_n^t$ and the relationship for the second order difference $\Delta^2 q_{n-1}^{t-1} = \Delta^2 q_n^{t-1} + O(\Delta x)^3$, $\Delta^2 q_{n+1}^{t-1} = \Delta^2 q_n^{t-1} + O(\Delta x)^3$ the above equation gives:

$$\frac{\Delta q_n^t}{\Delta t}\Delta t = (\Delta x)^2 \left\{ \frac{1}{4}\left(2\frac{\Delta^2 q_n}{(\Delta x)^2} + \frac{O(\Delta x)^3}{(\Delta x)^2} \right) \right\}^{t-\Delta t}$$

Taking the limits $\Delta x \to 0$, $\Delta t \to 0$, we obtain

$$\frac{\partial q}{\partial t} = \frac{1}{2} K_2 \frac{\partial^2 q}{\partial x^2} \tag{1.2}$$

Let $(\Delta x)^2 = (L_0/m)^2$ and $\Delta t = T_0/m^2$ then $K_2 = (\Delta x)^2/\Delta t = L_0{}^2/T_0$ where L_0, L_1 and T_0 are scale factors, $\Delta x = L_0/m$ and $\Delta t = T_0/m^2$ are element size and time interval respectively. Note that the derivation of the fundamental equation suggests that the time interval Δt for numerical calculation should me much smaller than the size adopted for the space elements Δx.

The classical diffusion coefficient is given by $D = K_2/2$. Equation (1.9) is the classical Fick´s equation for diffusion in isotropic media considering a single flux. There are other methods to derive this equation, as the random walk method inspired by the Brownian motion (Edelstein-Keshet, 1997; Zauderer, 1989).

As will be shown in the next chapter if we consider the retention process a new equation is obtained, namely a fourth order equation(Bevilacqua, et al. 2011a).;

$$\frac{\partial q}{\partial t} = \beta D \frac{\partial^2 q}{\partial x^2} - \beta(1-\beta) R \frac{\partial^4 q}{\partial x^4}$$

Note that we have now two terms on the right hand side suggesting that the process consists of two fluxes interconnected by the parameter β. If β=1, we recover the classical equation meaning that there is just one flux. For $\beta \neq 1$, secondary flux comes in. The discrete approach leads to an equation that describes nicely the presence of secondary flux in the diffusion process. A new constant R also appears automatically in the derivation process.

For the sake of completeness, it is interesting to say that for the case shown in Fig.1.2-a, if there is no retention the discrete approach leads to the classical wave equation:

$$\frac{\partial q}{\partial t} = -c\frac{\partial q}{\partial x}$$

Where *c* is the wave speed. Considering retention a new equation is obtained involving two fluxes as in the diffusion process and two new parameters β and K_3.

$$\frac{\partial q}{\partial t} = K_3\beta(1-\beta)\frac{\partial^3 q}{\partial x^3} - c\beta\frac{\partial q}{\partial x}$$

A more detailed discussion may be found in Bevilacqua et al. (2011a).

The main purpose of this thesis is to study the anomalous diffusion process that is governed by a fourth order equation, which will be derived using a discrete formulation similar as that presented above.

Given that the theory is new, several research branches are opened. The main purpose of this thesis is not to concentrate on a specific topic but to open the door for several research lines showing the challenges posed by this new theory. As a matter of fact as the analysis was in progress several questions came out which are new. So, one of the intentions of this work is to pose problems based on the case studies presented.

For the diffusion on a one-dimensional substratum, it is shown that negative value of the concentration develops after a pulse, Dirac function, at the origin. For mass transfer this behavior is only valid in the presence of a initial layer of material from which matter can be recruited. It was shown that the negative value of the solution appears only after a given slenderness of the initial conditions reached. This result opens a very interesting research field in mathematics. Also since the phenomenological considerations sustaining the theory require that the contents spreading on the given medium is homogeneous, that is, all particles are of the same nature the bi-flux appears due to the presence of different energy states. A short formulation of some fundamental hypothesis concerning energy distribution among the particles considering only kinetic energy is presented in chapter 6.

It was also derived the bi-flux diffusion equation for the plane. It is the simple case where the mass transfer for two orthogonal directions is the same. It is shown that the same type of singularity, or anomaly, with negative values of the concentration may appear at the corners of a rectangular domain.

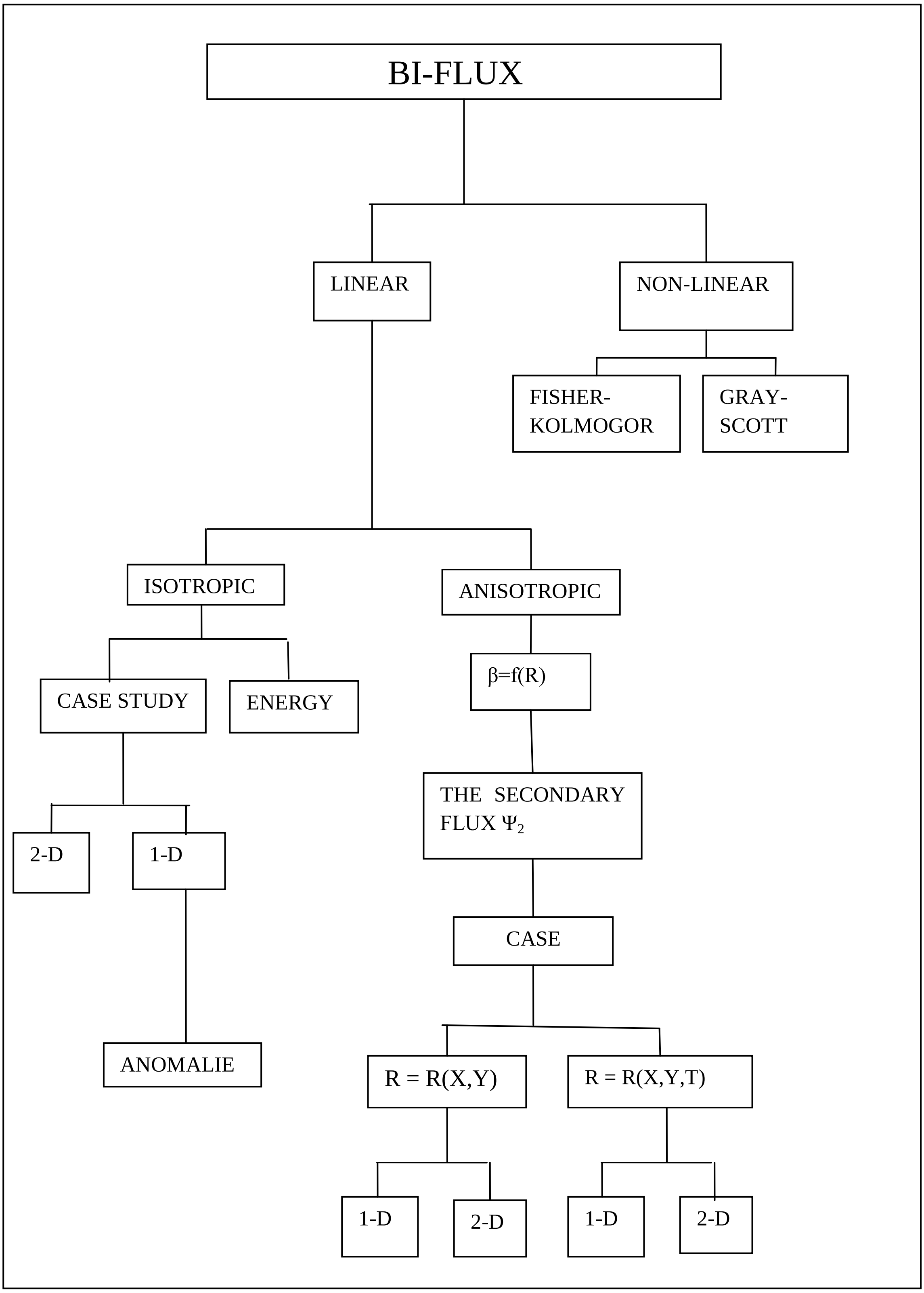
Most interesting is the case of diffusion in anisotropic media. Two new problems are posed. The first concerns the relationship between R and β. It has been suggested through the analysis of an inverse problems by Silva Neto et al. 2013, that these two coefficients are related. There is however no clue that could be used to propose a given relationship. The only restriction imposed by the fundamental hypothesis is that as R increases β should decrease. The second challenge is the definition of the secondary flux when the fraction β is function of x. A discussion of the influence of β(x) on the solution was presented. The influence of the definition of the secondary flux on the solution for anisotropic media is discussed through some examples. It was shown that for a given class of problems, after an initial particle distribution around the origin, the concentration increases instead of decreasing as expected. This phenomenon is related to the presence of a strong variation of R which apparently acts as an attractor. It is an acceptable process for the behavior of living organisms deployed on a medium with nutrients concentrated around a given point. The case with the reactivity coefficient R function of time for anisotropic media, that is $R=R(x,y,t)$ was also explored.

Finally two typical non-linear problems extensively discussed in the literature were also solved under the perspective of the bi-flux approach.

The flow chart below shows the connection among the several sections of the thesis. It is important to insist that the main contribution of this work is to open new research lines showing through numerical solutions the different types of behavior for the bi-flux diffusion process. Also the several possibilities opened for the behavior in anisotropic media depending on the relation $\beta=\mathrm{f}(R(x,y))$ and the on the definition of the secondary flux. It is also interesting the Gray-Scott problem regularization obtained with the bi-flux approach.

We think that the discussions on the influence of the reactivity constant R and the flux distribution β are important starting points for modeling several types of phenomenon particularly in biology. The solutions presented for some typical situations are stimulating for further analysis.

Finally it is important to say that the solution were developed with the Galerkin finite element method using Hermite polynomials for the fourth order equation and Lagrange polynomials when the fourth order equation is decomposed into two second order equations in the spatial space and the Euler backward difference in the temporal space. The nonlinear Galerkin finite element method is used to obtain the solution in the spatial space for non-linear case, also the Euler backward difference in the temporal space. Details on the numerical integration are presented in the appendix.


BI-FLUX
LINEAR
NON-LINEAR
FISHER-KOLMOGOR
GRAY-SCOTT
ISOTROPIC
ANISOTROPIC
CASE STUDY
ENERGY
β=f(R)
2-D
1-D
THE SECONDARY FLUX Ψ2
CASE
ANOMALIE
R = R(X,Y)
R = R(X,Y,T)
1-D
2-D
1-D
2-D

Chapter 2

The anomalous diffusion model and the bi-flux theory

2.1. Institution of the fundamental equations

Let us proceed as in the previous chapter. Consider the problem of diffusion in an isotropic medium. The discrete model is similar to the one introduced before except that now a fraction of the contents remains temporarily trapped in each cell while the remaining part is distributed equally to the right and to the left preserving symmetry in the distribution. Consider the same discretization as proposed before that is a sequence of m cells arranged in a chain along the x-axis Fig.2.1.

For the sake of completeness we will reproduce here the procedure introduced in Bevilacqua et al. (2011a). Let k represent the fraction retained at each time step. Consequently the remaining part $\beta = 1 - k$ will be equally distributed to the right and to the left cells. The corresponding discrete equations are (Bevilacqua et al., 2011a.):

$$q_n^t = kq_n^{t-1} + \frac{1}{2}(1-k)q_{n-1}^{t-1} + \frac{1}{2}(1-k)q_{n+1}^{t-1} \qquad (2.1\text{-a})$$

$$q_n^{t+1} = kq_n^t + \frac{1}{2}(1-k)q_{n-1}^t + \frac{1}{2}(1-k)q_{n+1}^t \qquad (2.1\text{-b})$$

Following the same procedure as in Bevilacqua *et al.* (2011a). let us introduce Eq.2.1-a into Eq.2.1-b to get:

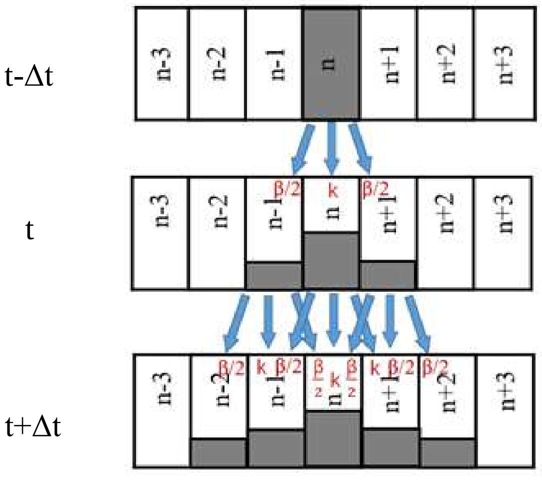


Fig.2.1. Diffusion with retention 1D case

$$\begin{aligned} q_n^{t+1} = k&\left[k q_n^{t-1} + \frac{1}{2}(1-k) q_{n-1}^{t-1} + \frac{1}{2}(1-k) q_{n+1}^{t-1} \right] + \\ &\frac{1}{2}(1-k)\left[k q_{n-1}^{t-1} + \frac{1}{2}(1-k) q_{n-2}^{t-1} + \frac{1}{2}(1-k) q_n^{t-1} \right] + \\ &\frac{1}{2}(1-k)\left[k q_{n+1}^{t-1} + \frac{1}{2}(1-k) q_n^{t-1} + \frac{1}{2}(1-k) q_{n+2}^{t-1} \right] \end{aligned}$$

Subtracting q_n^t given by Eq.2.1-a we get successively:

$$\begin{aligned} q_n^{t+1} - q_n^t &= -k(1-k) q_n^{t-1} + k(1-k)\left(q_{n-1}^{t-1} + q_{n+1}^{t-1}\right) - \\ &\frac{1}{2}(1-k)\left(q_{n-1}^{t-1} + q_{n+1}^{t-1}\right) + \frac{1}{4}(1-k)^2\left(q_{n-2}^{t-1} + 2q_n^{t-1} + q_{n+2}^{t-1}\right) \end{aligned} \tag{2.2-a}$$

$$\begin{aligned} q_n^{t+1} - q_n^t &= (1-k)\left[-\frac{1}{2}\left(q_{n-1}^{t-1} + q_{n+1}^{t-1}\right) + k\left(q_{n-1}^{t-1} + q_{n+1}^{t-1} + q_n^{t-1}\right) \right] + \\ &\frac{1}{4}(1-k)\left(q_{n-2}^{t-1} + 2q_n^{t-1} + q_{n+2}^{t-1}\right) \end{aligned} \tag{2.2-b}$$

$$\begin{aligned} q_n^{t+1} - q_n^t &= \frac{1}{4}(1-k)\left[q_{n-2}^{t-1} - 2q_{n-1}^{t-1} + 2q_n^{t-1} - 2q_{n+1}^{t-1} + q_{n+2}^{t-1}\right] + \\ &\frac{1}{4}(1-k)k\left[-q_{n-2}^{t-1} + 4q_{n-1}^{t-1} - 6q_n^{t-1} + 4q_{n+1}^{t-1} - q_{n+2}^{t-1}\right] \end{aligned} \tag{2.2-c}$$

$$\begin{aligned} q_n^{t+1} - q_n^t &= \frac{1}{4}(1-k)\left[\left(q_{n-2}^{t-1} - 2q_{n-1}^{t-1} + q_n^{t-1}\right) + \left(q_n^{t-1} - 2q_{n+1}^{t-1} + q_{n+2}^{t-1}\right)\right] + \\ &\frac{1}{4}(1-k)k\left[-q_{n-2}^{t-1} + 4q_{n-1}^{t-1} - 6q_n^{t-1} + 4q_{n+1}^{t-1} - q_{n+2}^{t-1}\right] \end{aligned} \tag{2.2-d}$$

From which follows the discrete form of the difference equation:

$$\Delta q_n^t = (1-k)\left\{ \frac{1}{4}\left[\Delta^2 q_n^{t-\Delta t} + O(\Delta x)^3\right] - \frac{1}{4} k \Delta^4 q_n^{t-\Delta t} \right\} \tag{2.2-e}$$

The Eq.2.2-e satisfies the requirements imposed by the limits of k, namely, k=0 classical diffusion and $k=1$ stationary solution. Rewriting Eq.2.2-e to get a finite difference equation we get:

$$\frac{\Delta q_n^{t+\Delta t}}{\Delta t}\Delta t = (1-k)\left\{-(\Delta x)^4 \frac{1}{4} k \frac{\Delta^4 q_n}{\Delta x^4} + (\Delta x)^2\left[\frac{1}{2}\frac{\Delta^2 q_n}{(\Delta x)^2} + \frac{O(\Delta x)^3}{(\Delta x)^2}\right]\right\}^{t-\Delta t}$$

Now with

$$\frac{(\Delta x)^2}{\Delta t} = \left(\frac{L_0}{m}\right)^2 \frac{m^2}{T_0} = \frac{L_0^{\ 2}}{T_0} \quad \frac{(\Delta x)^4}{\Delta t} = \left(\frac{L_1}{\sqrt{m}}\right)^4 \frac{m^2}{T_0} = \frac{L_1^4}{T_0}$$

where L_0, L_1 and T_0 are scale factors and $\Delta x = L_0/m = L_1/\sqrt{m}$,and $\Delta t = T_0/m$ are the cell size and the time interval respectively. Substituting these in the above relations, we obtain:

$$\frac{\Delta q_n^{t+\Delta t}}{\Delta t} = \frac{(1-k)}{2}\left\{\frac{L_0^2}{T_0}\left[\frac{\Delta^2 q_n}{\Delta x^2} + 2\frac{O(\Delta x)^3}{\Delta x^2}\right] - \frac{k}{2}\frac{L_1^4}{T_0}\frac{\Delta^4 q_n}{\Delta x^4}\right\}^{t-\Delta t} \tag{2.2-f}$$

with $K_2 = L_0^2/2T_0$, $K_4 = L_1^4/4T_0$ and if $q(x,t)$ is a sufficiently smooth function of x and t , such that $q(x,t) \in C^4$ we may take the limits as $\Delta x \to 0$ and $\Delta t \to 0$ to obtain:

$$\frac{\partial q}{\partial t} = (1-k)K_2 \frac{\partial^2 q}{\partial x^2} - k(1-k)K_4 \frac{\partial^4 q}{\partial x^4}$$

Now with $\beta = (1-k)$ and using the classical notation for the diffusion coefficient $K_2 = D$ and introducing a new coefficient $K_4 = R$ we get:

$$\frac{\partial q}{\partial t} = \beta D \frac{\partial^2 q}{\partial x^2} - \beta(1-\beta)R\frac{\partial^4 q}{\partial x^4} \tag{2.3}$$

The fourth order term with negative sign introduces the effect of retention. Clearly this term comes in naturally, without any artificial assumption, as an immediate consequence of the temporary retention imposed by the redistribution law. We would like to call the attention that similar equations can be obtained by introducing non-linear effects on the Fick's law (D'Angelo, 2003). These equations however are derived to consider other physical phenomena and hardly could be associated to the retention effect. The retention of the fraction (1− β) withtin the interval Δt generates the secondary flux. It is a kind of leaking effect at each time step Δt.

For the 2D case, we will follow a similar process to reach the fourth order model. Initially let us write the exchange relationship between the neighboring cells. We may write:

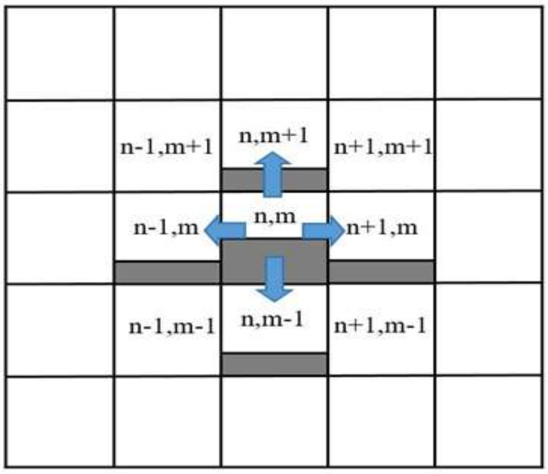


Fig.2.2. Diffusion with retention 2D case

$$q_{n,m}^{t} = kq_{n,m}^{t-1} + \frac{1}{4}(1-k)q_{n-1,m}^{t-1} + \frac{1}{4}(1-k)q_{n+1,m}^{t-1} + \frac{1}{4}(1-k)q_{n,m-1}^{t-1} + \frac{1}{4}(1-k)q_{n,m+1}^{t-1} \qquad (2.4\text{-a})$$

$$q_{n,m}^{t+1} = kq_{n,m}^{t} + \frac{1}{4}(1-k)q_{n-1,m}^{t} + \frac{1}{4}(1-k)q_{n+1,m}^{t} + \frac{1}{4}(1-k)q_{n,m-1}^{t} + \frac{1}{4}(1-k)q_{n,m+1}^{t} \qquad (2.4\text{-b})$$

Reducing the right hand side of equation (2.4-b) to time (t-1) leads successively to:

$$
\begin{aligned}
q_{n,m}^{t+1} = {} & k\left(kq_{n,m}^{t-1} + \frac{1}{4}(1-k)q_{n-1,m}^{t-1} + \frac{1}{4}(1-k)q_{n+1,m}^{t-1} + \frac{1}{4}(1-k)q_{n,m-1}^{t-1} + \frac{1}{4}(1-k)q_{n,m+1}^{t-1} \right) \\
& + \frac{1}{4}(1-k)\left(kq_{n-1,m}^{t-1} + \frac{1}{4}(1-k)q_{n-2,m}^{t-1} + \frac{1}{4}(1-k)q_{n,m}^{t-1} + \frac{1}{4}(1-k)q_{n-1,m-1}^{t-1} + \frac{1}{4}(1-k)q_{n-1,m+1}^{t-1} \right) \\
& + \frac{1}{4}(1-k)\left(kq_{n+1,m}^{t-1} + \frac{1}{4}(1-k)q_{n,m}^{t-1} + \frac{1}{4}(1-k)q_{n+2,m}^{t-1} + \frac{1}{4}(1-k)q_{n+1,m-1}^{t-1} + \frac{1}{4}(1-k)q_{n+1,m+1}^{t-1} \right) \\
& + \frac{1}{4}(1-k)\left(kq_{n,m-1}^{t-1} + \frac{1}{4}(1-k)q_{n-1,m-1}^{t-1} + \frac{1}{4}(1-k)q_{n+1,m-1}^{t-1} + \frac{1}{4}(1-k)q_{n,m-2}^{t-1} + \frac{1}{4}(1-k)q_{n,m}^{t-1} \right) \\
& + \frac{1}{4}(1-k)\left(kq_{n,m+1}^{t-1} + \frac{1}{4}(1-k)q_{n-1,m+1}^{t-1} + \frac{1}{4}(1-k)q_{n+1,m+1}^{t-1} + \frac{1}{4}(1-k)q_{n,m}^{t-1} + \frac{1}{4}(1-k)q_{n,m+2}^{t-1} \right)
\end{aligned}
$$

Simplifying the equation above, we can obtain:

$$
\begin{aligned}
q_{n,m}^{t+1} = {} & k^2 q_{n,m}^{t-1} + 2\frac{k(1-k)}{4}\left(q_{n-1,m}^{t-1} + q_{n+1,m}^{t-1} + q_{n,m-1}^{t-1} + q_{n,m+1}^{t-1} \right) \\
& + \frac{(1-k)^2}{16}\left(q_{n-2,m}^{t-1} + q_{n,m}^{t-1} + q_{n-1,m-1}^{t-1} + q_{n-1,m+1}^{t-1} \right) \\
& + \frac{(1-k)^2}{16}\left(q_{n,m}^{t-1} + q_{n+2,m}^{t-1} + q_{n+1,m-1}^{t-1} + q_{n+1,m+1}^{t-1} \right) \\
& + \frac{(1-k)^2}{16}\left(q_{n-1,m-1}^{t-1} + q_{n+1,m-1}^{t-1} + q_{n,m-2}^{t-1} + q_{n,m}^{t-1} \right) \\
& + \frac{(1-k)^2}{16}\left(q_{n-1,m+1}^{t-1} + q_{n+1,m+1}^{t-1} + q_{n,m}^{t-1} + q_{n,m+2}^{t-1} \right)
\end{aligned}
$$

Subtracting $q_{n,m}^{t}$ given by (2.4-a), we get successively:

$$
\begin{aligned}
q_{n,m}^{t+1} - q_{n,m}^{t} = {} & -k(1-k)q_{n,m}^{t-1} + \frac{k(1-k)}{2}\left(q_{n-1,m}^{t-1} + q_{n+1,m}^{t-1} + q_{n,m-1}^{t-1} + q_{n,m+1}^{t-1} \right) - \frac{1-k}{4}\left(q_{n-1,m}^{t-1} + q_{n+1,m}^{t-1} + q_{n,m-1}^{t-1} + q_{n,m+1}^{t-1} \right) \\
& + \frac{(1-k)^2}{16}\left[\left(q_{n-2,m}^{t-1} + 2q_{n,m}^{t-1} + q_{n+2,m}^{t-1} \right) + \left(q_{n,m+2}^{t-1} + 2q_{n,m}^{t-1} + q_{n,m+2}^{t-1} \right) + 2\left(q_{n-1,m-1}^{t-1} + q_{n+1,m-1}^{t-1} + q_{n-1,m+1}^{t-1} + q_{n+1,m+1}^{t-1} \right) \right]
\end{aligned}
$$

Or

$$
\begin{aligned}
&= \frac{(1-k)}{16}\left[-4\left(q_{n-1,m}^{t-1} + q_{n+1,m}^{t-1} + q_{n,m-1}^{t-1} + q_{n,m+1}^{t-1}\right)\right] \\
&+ \frac{(1-k)}{16}\left(q_{n-2,m}^{t-1} + 2q_{n,m}^{t-1} + q_{n+2,m}^{t-1} + q_{n,m+2}^{t-1} + 2q_{n,m}^{t-1} + q_{n,m+2}^{t-1} + 2q_{n-1,m-1}^{t-1} + 2q_{n+1,m-1}^{t-1} + 2q_{n-1,m+1}^{t-1} + 2q_{n+1,m+1}^{t-1}\right) \\
&+ \frac{(1-k)k}{16}\left[8\left(q_{n-1,m}^{t-1} - q_{n,m}^{t-1} + q_{n+1,m}^{t-1} + q_{n,m-1}^{t-1} - q_{n,m}^{t-1} + q_{n,m+1}^{t-1}\right)\right] \\
&- \frac{(1-k)k}{16}\left(q_{n-2,m}^{t-1} + 2q_{n,m}^{t-1} + q_{n+2,m}^{t-1} + q_{n,m+2}^{t-1} + 2q_{n,m}^{t-1} + q_{n,m+2}^{t-1} + 2q_{n-1,m-1}^{t-1} + 2q_{n+1,m-1}^{t-1} + 2q_{n-1,m+1}^{t-1} + 2q_{n+1,m+1}^{t-1}\right)
\end{aligned}
$$

On the right side of the equation, rearrange each term to lead to the sum of several convenient difference terms

$$
\begin{aligned}
q_{n,m}^{t+1} - q_{n,m}^{t} &= \frac{(1-k)}{16}\left[\left(q_{n,m-2}^{t-1} - 2q_{n,m-1}^{t-1} + q_{n,m}^{t-1}\right) + \left(q_{n-1,m-1}^{t-1} - 2q_{n,m-1}^{t-1} + q_{n+1,m-1}^{t-1}\right)\right] \\
&+ \frac{(1-k)}{16}\left[\left(q_{n,m}^{t-1} - 2q_{n,m+1}^{t-1} + q_{n,m+2}^{t-1}\right) + \left(q_{n-1,m+1}^{t-1} - 2q_{n,m+1}^{t-1} + q_{n+1,m+1}^{t-1}\right)\right] \\
&+ \frac{(1-k)}{16}\left[\left(q_{n+1,m-1}^{t-1} - 2q_{n+1,m}^{t-1} + q_{n+1,m+1}^{t-1}\right) + \left(q_{n,m}^{t-1} - 2q_{n+1,m}^{t-1} + q_{n+2,m}^{t-1}\right)\right]
\end{aligned}
$$

$$
\begin{aligned}
&+ \frac{(1-k)}{16}\left[\left(q_{n,m}^{t-1} - 2q_{n-1,m}^{t-1} + q_{n-2,m}^{t-1}\right) + \left(q_{n-1,m-1}^{t-1} - 2q_{n-1,m}^{t-1} + q_{n-1,m+1}^{t-1}\right)\right] \\
&- \frac{(1-k)k}{16}\left(q_{n-2,m}^{t-1} - 4q_{n-1,m}^{t-1} + 6q_{n,m}^{t-1} - q_{n+1,m}^{t-1} + q_{n+2,m}^{t-1}\right) \\
&- \frac{(1-k)k}{16}\left(q_{n,m-2}^{t-1} - 4q_{n,m-1}^{t-1} + 6q_{n,m}^{t-1} - q_{n,m+1}^{t-1} + q_{n,m+2}^{t-1}\right) \\
&- \frac{2(1-k)k}{16}\left[\left(q_{n-1,m-1}^{t-1} - 2q_{n-1,m}^{t-1} + q_{n-1,m+1}^{t-1}\right) - 2\left(q_{n,m-1}^{t-1} - 2q_{n,m}^{t-1} + q_{n,m+1}^{t-1}\right) + \left(q_{n+1,m-1}^{t-1} - 2q_{n+1,m}^{t-1} + q_{n+1,m+1}^{t-1}\right)\right]
\end{aligned}
$$

Then, recall

$$q_{n,m}^{t+1} - q_{n,m}^{t} = \Delta q_{n,m}^{t},$$

$$q_{n-1,m-1}^{t-1} - 2q_{n,m-1}^{t-1} + q_{n+1,m-1}^{t-1} = \Delta_y^2 q_{n,m-1}^{t-1}$$

$$q_{n-1,m-1}^{t-1} - 2q_{n,m-1}^{t-1} + q_{n+1,m-1}^{t-1} = \Delta_x^2 q_{n,m-1}^{t-1}$$

for the cell $(n, m-1)$. For the other cells, the equation is very similar except for the corresponding cells indices. With the above notation the equation will be written as:

$$\Delta q_{n,m}^{t} = \frac{(1-k)}{16}\left[\Delta_y^2 q_{n,m-1}^{t-1} + \Delta_x^2 q_{n,m-1}^{t-1} + \Delta_y^2 q_{n,m+1}^{t-1} + \Delta_x^2 q_{n,m+1}^{t-1} + \Delta_y^2 q_{n,m}^{t-1} + \Delta_x^2 q_{n+1,m}^{t-1} + \Delta_y^2 q_{n-1,m}^{t-1} + \Delta_x^2 q_{n-1,m}^{t-1}\right]$$
$$-\frac{(1-k)k}{16}\left[\Delta_x^4 q_{n,m}^{t-1} + \Delta_y^4 q_{n,m}^{t-1} - 2\Delta_y^2\left(\Delta_x^2 q_{n,m}^{t-1}\right)\right]$$

Adding similar terms the equation is reduced to:

$$\Delta q_{n,m}^{t} = \frac{(1-k)}{4}\left[\Delta_x^2 q_{n,m}^{t-1} + \Delta_y^2 q_{n,m}^{t-1} + O\left((\Delta x)^3 + (\Delta y)^3\right)\right] - \frac{(1-k)k}{16}\left[\Delta_x^4 q_{n,m}^{t-1} + \Delta_y^4 q_{n,m}^{t-1} + 2\Delta_y^2\left(\Delta_x^2 q_{n,m}^{t-1}\right)\right]$$

Rewriting the equation above to obtain a finite difference form of a differential equation we will get:

$$\frac{\Delta q_{n,m}^{t+\Delta t}}{\Delta t}\Delta t = \left(\frac{(1-k)}{4}(\Delta s)^2\left(\frac{\Delta_{x^2}^2 q_{n,m}^{t-1} + \Delta_y^2 q_{n,m}^{t-1}}{(\Delta s)^2} + \frac{O\left((\Delta x)^3 + (\Delta y)^3\right)}{(\Delta s)^2}\right)\right)^{t-\Delta t} -$$
$$-\left(\frac{(1-k)k}{16}(\Delta s)^4\,\frac{\Delta_x^4 q_{n,m}^{t-1} + \Delta_y^4 q_{n,m}^{t-1} + 2\Delta_y^2\left(\Delta_x^2 q_{n,m}^{t-1}\right)}{(\Delta s)^4}\right)^{t-\Delta t}$$

Where, $\Delta s = \Delta x = \Delta y$

Take the limits as $\Delta s \to 0$, $\Delta t \to 0$, we obtain

$$\frac{\partial q}{\partial t} = \beta D \Delta q - \beta(1-\beta) R \Delta(\Delta q) \qquad (2.9)$$

where *β, D, R* represent, respectively, the fraction of elements in the primary flux, the diffusion coefficient and the reactivity coefficient. The coefficients *D* and *R* are the limiting values of $\lim_{\Delta s,\Delta t \to 0} (\Delta s)^2 / (4\Delta t)$ and $\lim_{\Delta s,\Delta t \to o} (\Delta s)^4 / (16\Delta t)$. The Eq. 2.9 is the anomalous diffusion model for a two dimensional domain. For $\beta = 0$, the system becomes stationary, and for $\beta = 1$, the system reduces to the classical diffusion model in two dimensions.

2.2. The Bi-flux theory

The results obtained from the discrete approach for 1-D and 2-D strongly suggest the existence of a secondary flux corresponding to the fourth order derivative of the concentration. With the presence of the secondary flux the mass conservation principle leads to an equation valid for a continuum. Now it is not difficult to propose a new law for the secondary flux. Indeed, the generalization of the proposition advanced in Bevilacqua *et al*. (2013), for a two dimensional domain reads:

PROPOSITION: *Suppose a two-dimensional diffusion process consisting of N particles moving in a homogeneous, isotropic supporting medium according to the Fick´s law. If a fraction* $f(N) = (1-\beta)$ *of the diffusing particles is temporarily delayed along their trajectories due to some mechanical,biological, physical, chemical or physicochemical interaction with the medium, that doesn't disturb the diffusion coefficient D, the governing equation must include a fourth order differential term of the form:*

$$-\beta(1-\beta)R\Delta(\Delta q(x,y,t))$$

where R *is a material constant, β the fraction of the particles in the Fickian or primary flux, with* $0 < \beta \leq 1$ *constant, and* $q(x,y,t)$*stands for the particle concentration in the medium.*

The operator Δ is $\Delta(\ ) = \frac{\partial^2(\ )}{\partial x^2} + \frac{\partial^2(\ )}{\partial y^2}$ for a two dimensional domain.

For one dimensional problem $\Delta(\Delta q) = \frac{\partial^4 q}{\partial x^4}$

Before stating the laws that govern retention it is worthwhile describing some basic ideas sustaining the formulation that will be introduced later on. Scientists and particularly engineers have frequently to deal with a class of problems that behind an apparent simplicity hide complex events. A problem with hidden complexity results from the simultaneous convergence of several phenomena involving a relatively large number of transformation processes. Most of the problems belonging to that class appearing in engineering practice require the determination of certain variables, that we will call here macro-state variables, representing complex physical, chemical or physicochemical interactions at micro scales. For the engineering point of view, within certain limits, it is not necessary to analyze the phenomenon at the smallest possible scale, since often the basic phenomena are not yet fully understood. It suffices knowing the behavior of the macro-state variables. That is, for a problem with hidden complexity, in several circumstances, the main task is to determine the relationship among the input variables and the output variables flowing in and out of a "black box". As a matter of fact the microstate phenomena related to the classical diffusion problem has been analyzed in detail since the beginning of the last century with the pioneering works of Einstein (1905) and Smoluchowski (1916).

The delayed diffusion process however requires the introduction of an extended energy state where the kinetic energy may include the spin energy of the particles which are not considered in the classical theories as far as we know. Only recently, particularly with the observation of fluctuations in the diffusion processes (Bustamante, et al. 2005) and the presence of self-excited particles, new theories are taken into consideration (Riedel, et al. 2015). The determination of a method or a theory adequate to establish the behavior of the macro-variables is by no means an easy task. The main difficulty arises from the fact that the theory must play a unification role. That is, the theory must as far as possible translate with a relatively simple set of rules and laws the response of the macro-state variables to the perturbations introduced in the system under consideration. More than that, a successful theory should give adequate response to several similar phenomena belonging to the same class. For instance, dispersion of gas, liquid or solid particles in different supporting media should be accurately modeled by the same theoretical framework because they belong to the same class of problems independently of the particle nature and of the medium. The macro-variable for this class of phenomenon is the particle concentration denoted by $q(\mathrm{x},t)$. The theory proposed in this paper is derived from the following ideal process:

Consider a collection of particles immersed in some medium and moving in a preferred direction driven by repulsion forces such that they displace from high concentration regions towards low concentration regions free from constraints. The motion is not subjected to any critical barrier that could induce a significant perturbation in the process. Under this circumstance it is plausible to admit that the average speed of the particles is proportional to the concentration gradient, the particles being driven from regions with high concentration levels, strong repulsive forces, to regions with low concentration levels, weak repulsive forces. This is the fundamental idea supporting Fick´s law. For the one dimensional problem in a homogeneous medium the absolute value of the diffusion speed may be defined as $D\partial q(x,t)/\partial x$ where D is the diffusion coefficient.

The diffusion coefficient cannot be considered as a parameter characterizing a single well defined physicochemical phenomenon. It is instead a coefficient associate to an ideal event that simulates satisfactorily a wide range of phenomena. The diffusion coefficient may have different physical interpretations depending on the particular phenomenon under consideration. Another way to see this methodology is to consider a “black box” that transforms input variables into output variables according to well established laws irrespectively from the physics that may be going on inside the box. In this sense the Fick´s law is a des-complexification process. Note that we are also considering the diffusion process at large including, for example, knowledge diffusion and capital flow.

Now suppose that other events interfere in the diffusion mechanism. In this case the law must be modified accordingly. For instance, the effects of sources or sinks in a diffusion process cannot be modeled by some artificial modification of the flow velocity or distorting the interpretation of the diffusion coefficient. A new term is necessary to be incorporated in the governing equation. Diffusion with sinks or sources belongs to a different class of phenomena.

To avoid possible misunderstandings referring to more complex diffusion problems, we would like to remark that it is possible within a same class of phenomena to improve the respective laws incorporating extra terms. For the case of diffusion, for instance, Fick´s law may be extended to incorporate non-linear terms adjusting theoretical results better to more accurate observations. This means that the driving forces inducing the particles motion cannot be related only to the gradient of the concentration but requires the consideration of higher order terms. This is a refinement of the theoretical framework, but the basic event remains the same, belonging to the class of diffusion problems without taking into account any other phenomenon as retention for instance.

If however there is some essential modification of the phenomenology governing a given process, it is necessary to review the theoretical framework to find some universal model adequate to des-complexify the corresponding class of phenomenon. Unfortunately, not seldom, it is found in the literature attempts to extend a theory fitted to represent a given class of events to a new phenomenological class. The results are certainly not universal and may fail to express a reliable response of the macro-state variables. This is the case of diffusion with delaying effect. Delay in the diffusion process cannot be adequately modeled by Fick´s law or any refinement of the classical diffusion law. Diffusion with delay, provided that the diffusion coefficient remains constant, belongs to another class of phenomena. A new suitable law could be stated axiomatically. Better would be to find a kind of universal event that may encompass a large number of phenomena and provide a consistent evaluation of the macro-state variables.

2.2.1. The secondary flux and the mass conservation principle

The results obtained up to now in our investigation allow for the introduction of a new scattering law. We have already seen that the discrete approach introduces a fourth order term in the classical diffusion equation. Now this term can be associated to a secondary flux. Indeed the retained fraction of particles $(1-\beta)$remains in the cell n for a small time interval Δt. After this period of time there is a different amount of particles retained in the same cell n. This means that the successive change in contents of a general cell n induces an evolutionary process associated to the retention assumption. Therefore, it is plausible to assume that the fourth order term is associated to a secondary flux. Following the similar assumption taken to introduce the Fick´s law that is:

$$\boldsymbol{\Psi}_1 = -D\frac{\partial q(x,t)}{\partial x}\mathbf{e}_x \qquad (2.10\text{-a})$$

We may write for the secondary flux (Bevilacqua *et al*. 2013),

$$\boldsymbol{\Psi}_2 = R\beta\frac{\partial^3 q(x,t)}{\partial x^3}\mathbf{e}_x \qquad (2.10\text{-b})$$

Where $\mathbf{e}_x$ is unit vector for the x axis. This proposal was first put forward in Bevilacqua *et al*. (2013). We assume here that we have an isotropic process, that is, all parameters are independent of x and y in a two dimensional domain. We will discuss later in chapter 3 the case for anisotropic media.

For this case, the expression for the first flux, obeying the Fick´s law, can be written as:

$$\boldsymbol{\Psi}_1 = -D\nabla q(x,y,t) \quad \text{with} \quad \nabla(\ ) = \frac{\partial(\ )}{\partial x}\mathbf{e}_\mathbf{x} + \frac{\partial(\ )}{\partial y}\mathbf{e}_y$$

The secondary flux is not well defined a priori by the results obtained with the discrete approach. Although for isotropic media the order of the differential operator is not important, it will make a crucial difference for anisotropic media. Therefore we introduce here three possible expressions:

$$\boldsymbol{\Psi}_2^1 = R(x,y,t)\beta\nabla(\Delta q(x,y,t))$$

$$\boldsymbol{\Psi}_2^2 = R(x,y,t)\nabla(\beta\Delta q(x,y,t))$$

$$\boldsymbol{\Psi}_2^3 = R(x,y,t)\nabla(\nabla\cdot(\beta\nabla q(x,y,t)))$$

$$\text{with } \Delta(\ ) = \frac{\partial^2(\ )}{\partial x^2} + \frac{\partial^2(\ )}{\partial y^2}$$

The equations above show clearly the existence of two different diffusion processes. From the Eq.2.9, it is possible to see that particles belonging to the fraction β follow the classical Fick´s law, it is the primary flux that is called $\boldsymbol{\Psi}_1$ and particles belonging to the fraction (1−β) follow a new law, it is the secondary flux that is called $\boldsymbol{\Psi}_2^i, i = 1,2,3$.

Now with the considerations above it is possible to derive the generalized equation from the classical mass conservation principle. Indeed if we assume the two laws for the flux rates with $\boldsymbol{\Psi}_1$ corresponding to the fraction of particles β diffusing according to Fick´s law and $\boldsymbol{\Psi}_2^i, i = 1,2,3$ ruling the complementary fraction (1−β), the mass conservation principle gives:

$$\int_V \frac{q(\mathbf{x}, t+\Delta t) - q(\mathbf{x}, t)}{\Delta t} ds + \int_{\partial V} \left[\beta \boldsymbol{\Psi}_1 + (1-\beta)\boldsymbol{\Psi}_2^i\right] \cdot \left[\mathbf{e}_x, \mathbf{e}_y\right] ds = 0$$

D is the diffusion coefficient and R we call reactivity coefficient. Both in general may be functions of $\mathbf{x}$ an t. And for $\mathbf{x} \in R^2$:

$$\frac{\partial q}{\partial t} = \nabla \cdot (\beta D \nabla q) - \nabla \cdot (R\beta(1-\beta)\nabla(\Delta q)) \tag{2.12a}$$

$$\frac{\partial q}{\partial t} = \nabla \cdot (\beta D \nabla q) - \nabla \cdot (R(1-\beta)\nabla(\beta \Delta q)) \tag{2.12b}$$

$$\frac{\partial q}{\partial t} = \nabla \cdot (\beta D \nabla q) - \nabla \cdot (R(1-\beta)\nabla(\nabla \cdot (\beta \nabla q))) \tag{2.12c}$$

The physical meaning of the primary flux is well known, namely, the particle concentration distribution tends to smooth out along the space variable. The particles move from higher concentration regions toward lower concentration regions. The secondary flux is concerned with the curvature variation of the concentration distribution. Recall that the curvature of the function $q(x,t)$ is proportional to the second derivative $\left(\partial^2 q / \partial x^2\right)$ of the concentration. Therefore the secondary flux grows with the variation of the second derivative.

In this section we have represented the one dimensional equation and utilizing the same discrete method have derived one two dimension model intended to describe anomalous diffusion processes. The next section is devoted to the investigation of some simple examples. Initially we will consider all the parameters constant.

It is convenient at this stage to make some comments regarding the boundary conditions. Four boundary conditions are necessary to define the problem on a finite domain. There are four kinds of boundary conditions. Three are easy to understand, namely:

1. The value of the concentration $q(x,y,t)\big|_{\bar{x},\bar{y}} = \bar{q}$

2. The primary flux $\mathbf{\Psi}_1(x,y,t)\big|_{\bar{x},\bar{y}} = \overline{\mathbf{\Psi}}_1$

3. The secondary flux $\mathbf{\Psi}_2(x,y,t)\big|_{\bar{x},\bar{y}} = \overline{\mathbf{\Psi}}_2$

The fourth acceptable boundary condition is related to the second derivative of the concentration. It is admissible, at least theoretically to impose as boundary condition:

$$\Delta q(x,y,t)\big|_{\bar{x},\bar{y}} = \Delta\bar{q}$$

The physical interpretation is still not completely clarified. However from the results that we have obtained, and will be presented in the sequel, this condition is related to the curvature of the concentration profile. At least for one case related to the deposition of thin films, molecular beam epitaxy (MBE) (Barabási *et al.* 1995) the curvature plays a key role in the process. For our problem the role of the curvature needs to be further explored although there are indications that particles may tend to converge to regions with higher curvature in anisotropic media.

2.3 Test of the numerical solution

The development of this work is strongly dependent on the numerical solution of the fourth order partial differential equation for the bi-flux theory. Therefore it is convenient to present the solution for a fundamental case with brief description of the method used and a convergence test. Let us consider the equation:

$$\frac{\partial q(x,y,t)}{\partial t} = \nabla\cdot\left(\beta D\nabla q(x,y,t)\right) - \nabla\cdot\left(\beta(1-\beta)R\nabla\left(\Delta q(x,y,t)\right)\right) \tag{2.13}$$

The variable q(x,y,t) is defined in $\Omega\subset[-1,1]\mathrm{x}[-1,1]$. The diffusion coefficient is D=0.1, the reactivity coefficient is R=0.01, and the primary fraction β=0.33. The boundary conditions are:

$\nabla q.\mathbf{n}\big|_{\partial\Omega} = 0$ and $\nabla\Delta q.\mathbf{n}\big|_{\partial\Omega} = 0$

The initial condition is given by:

$q(x,y,0)=\cos(\pi x)\cos(\pi y)$

The problem has an analytical solution namely:

$q(x,y,t)=e^{-1.515t}\cos(\pi x)\cos(\pi y)$

First we reduce the fourth order problem to two coupled second order equations. Introducing a new variable $p(x,y,t)=\Delta q(x,y,t)$ the equation (2.13) can be substituted by the system:

$$\begin{cases} \dfrac{\partial q(x,y,t)}{\partial t}=\beta D\Delta q(x,y,t)-\beta(1-\beta)R\Delta(p(x,y,t)) \\ \qquad\qquad p(x,y,t)=\Delta q(x,y,t) \end{cases}$$

With the initial and boundary conditions:

$q(\mathbf{x},0)=q_0(\mathbf{x})$ $\qquad\mathbf{x}\in\Omega$

$p(\mathbf{x},0)=\Delta q(\mathbf{x},0)=\Delta q_0(\mathbf{x})$ $\qquad\mathbf{x}\in\Omega$

$\nabla q(\mathbf{x},t)=0\,,\nabla p(\mathbf{x},t)=0$ on the boundaries

The solution was obtained with the finite elements method. The mesh is composed by quadrangular elements leading to a conformal finite element formulation. Note that all 2-D problems solved in this thesis are defined on a domain (LxL). The base functions are the cubic Hermite polynomials composing the finite element approximation of Bogner-Fox-Schmidt (BFS) (Bogner, Fox, and Schmit, 1965). Using the Galerkin method to derive the mass [M] and stiffness [K] matrices associated to the variables vectors

$$Q=\left[q^1,q_x^1,q_y^1,q_{xy}^1\cdots,q^{n+1},q_x^{n+1},q_y^{n+1},q_{xy}^{n+1}\right]$$

$$P=\left[p^1,p_x^1,p_y^1,p_{xy}^1\cdots,p^{n+1},p_x^{n+1},p_y^{n+1},p_{xy}^{n+1}\right]$$

It is obtained the system:

$$\begin{bmatrix} M+\Delta t\beta D\cdot K & -\Delta t\beta(1-\beta)R\cdot K \\ K & M \end{bmatrix}\begin{bmatrix} Q \\ P \end{bmatrix}^{t+1}=\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} Q \\ P \end{bmatrix}^{t}$$

For time integration, the Euler backward difference was used to approximate the solution q(x,y,t) and p(x,y,t). With the initial conditions Q^0 and P^0 for $t=0$ the solution can be obtained with the platform Matlab.

With the cubic Hermite polynomials (Chien, *et al*. 2009; Ruckert, 2013) it is possible to obtain the approximation of the functions q(x,y,t) and p(x,y,t) with good accuracy and higher order derivatives as well. Firstly, some mathematic definitions of the numerical development are represented as below,

For the one dimensional case the reference interval $I = [-1,1]$ is divided into elements of equal size, $N_i = 5;10;20;40;80$ elements succesviley leading to:

$h_i = 2/N_i$, $i = 1,...,5.$

The order of convergence for the numerical method has been computed by the expression:

$$Order = \log\left(\left\|u - u_{h_i}\right\|_{L^j} / \left\|u - u_{h_{i+1}}\right\|_{L^j}\right) / \log(2),\ i = 1,...,5.,\ j = 2, \infty .$$

Where u_{h_i} is the numerical solution with step size h_i, while $h_{i+1} = h_i/2$.

$$\left\|u - u_h\right\|_{L^2} = \sqrt{\sum_{s=1}^{N} h\left|u_s - u(x_s)\right|^2}\ ,\ \left\|u - u_h\right\|_{L^\infty} = \max_s \left|u_s - u(x_s)\right|$$

Where u denotes the exact solution and u_s is the numerical solution on the sth node in the mesh u_h, N is the total number of nodes in the mesh u_h. For the two dimensional case, consider the reference domain, $\Omega = [-1,1] \times [-1,1]$

$$\left\|u - u_h\right\|_{L^2} = \sqrt{\sum_{s=1}^{N} h_x h_y \left|u_s - u(x_s)\right|^2}$$

h_x is the length for subdomain on *x* axis, h_y is the length for subdomain on *y* axis. The tables below (2.1a,b,c) show the errors in the L_∞ and L_2 norms for $q(x,y,t)$ the first and third derivatives.

Table 2.1a CPU time, error and order of accuracy of $q(x,y,t)$ with BFS element

N	h	Δt	CPU(s)	L_∞ for q	Order	L_2 for q	Order
5*5	0.2	4.00e(-2)	0.49	2.37e(-2)	----	1.66e(-2)	----
10*10	0.1	1.00e(-2)	2.00	5.90e(-3)	2.01	3.50e(-3)	2.25
20*20	0.05	2.50e(-3)	22.66	1.50e(-3)	1.98	8.05e(-4)	2.12
40*40	0.025	6.25e(-4)	505.94	3.66e(-4)	2.04	1.90e(-4)	2.08
80*80	0.0125	1.56e(-4)	12418.23	9.14e(-5)	2.00	4.68e(-5)	2.03

Final time T=1.0

Table 2.1b CPU time, error and order of accuracy of $q_x(x,y,t)$ with BFS element

N	h	Δt	CPU(s)	L_∞ for q_x	Order	L_2 for q_x	Order
5*5	0.2	4.00e(-2)	0.49	7.16e(-2)	----	4.45e(-2)	----
10*10	0.1	1.00e(-2)	2.00	1.85e(-2)	1.95	1.01e(-2)	2.14
20*20	0.05	2.50e(-3)	22.66	4.60e(-3)	2.01	2.40e(-3)	2.07
40*40	0.025	6.25e(-4)	505.94	1.10e(-3)	2.06	5.85e(-4)	2.04
80*80	0.0125	1.56e(-4)	12418.23	2.87e(-4)	1.94	1.45e(-4)	2.01

Final time T=1.0

Table 2.1c CPU time, error and order of accuracy of $q_{xxx}(x,y,t)$ with BFS element

N	h	Δt	CPU(s)	L_∞ for q_{xxx}	Order	L_2 for q_{xxx}	Order
5*5	0.2	4.00e(-2)	0.49	1.41	----	8.77e(-1)	----
10*10	0.1	1.00e(-2)	2.00	3.65e(-1)	1.95	2.00e(-1)	2.13
20*20	0.05	2.50e(-3)	22.66	9.08e(-2)	2.01	4.76e(-2)	2.07
40*40	0.025	6.25e(-4)	505.94	2.27e(-2)	2.00	1.16e(-2)	2.04
80*80	0.0125	1.56e(-4)	12418.23	5.70e(-3)	2.00	2.90e(-3)	2.00

Final time T=1.0

The convergence order for the Hermite cubic element is approximately equal 2 for the function, the first and second derivatives. The CPU time increases exponentially with no expressive gain in the approximation. Therefore it is convenient to define the maximum admissible error to reduce the costs in computer time.

Fig.2.3a,b show the errors for the function and its first and second derivatives in the L_∞ and L_2 norms. The higher the derivative order the higher is the error as expected. In any case the errors are small indicating that the method leads to a good approximation.

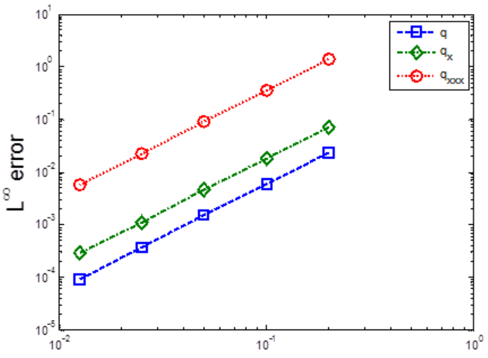


Fig.2.3a h vs L_∞ error

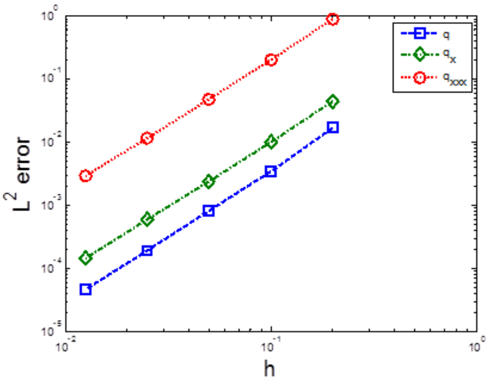


Fig.2.3b h vs L_2 error

If we don't need the approximations for higher order derivatives it is possible to use the first order bilinear Lagrange polynomials as base functions. The errors in L_∞ and L_2 norms are shown in table 2.2.

Table 2.2 CPU time, error and order of accuracy of q with Lagrange element

N	h	Δt	CPU(s)	L_∞ for q	Order	L_2 for q	Order
5*5	0.2	4.00e(-2)	0.07	6.90e(-3)	----	4.80e(-3)	----
10*10	0.1	1.00e(-2)	0.23	1.60e(-3)	2.11	9.49e(-4)	2.34
20*20	0.05	2.50e(-3)	2.31	3.94e(-4)	2.02	2.17e(-4)	2.13
40*40	0.025	6.25e(-4)	35.76	9.81e(-5)	2.01	5.15e(-5)	2.08
80*80	00125	1.56e(-4)	652.00	2.45e(-5)	2.00	1.25e(-5)	2.04

Final time T=1.0

The convergence order for L_∞ and L_2 are similar to the results obtained with the cubic Hermite element. The CPU time is drastically reduced. So if only the value of the function is required, the non-conforming element derived with the Lagrange base functions may lead to a considerable spare in computer time. This is however only possible under the condition of non-flux at the boundaries. The Fig.2.4a,b show the variation of the errors with the element size. The convergence in the L_2 norm is slightly superior compared to the convergence in L_∞.

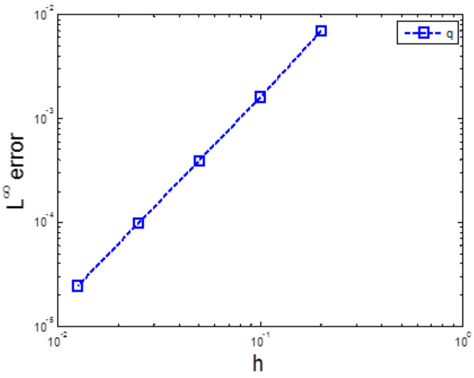


Fig.2.4a h vs L_∞ error

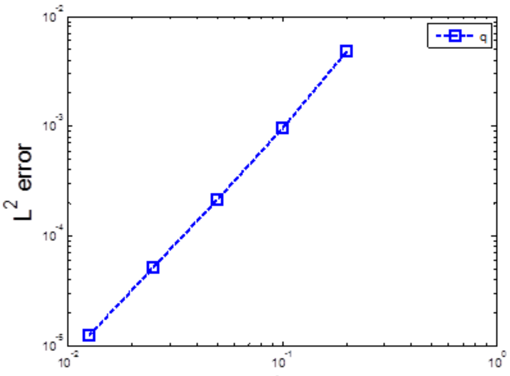


Fig.2.4b h vs L_2 error

This test can said to be a good base to accredit the method to be used for the next problems. For the bi-flux diffusion problem in anisotropic media the mass and stiffness matrices become more complex and it is necessary integration operations considering the coefficients R and β as function of the space variables. We will consider D constant in the problems discussed here.

Chapter 3

Isotropic diffusion processes

This section deals with the behavior of some solutions for isotropic diffusion problems with time independent parameters to investigate possible deviations from the classical approach. That is in which extent the fourth order term perturbs the classical solutions. The following two cases are elementary from the analytical point of view but very illustrative concerning some possible physical mechanism triggered by the bimodal diffusion process. It will be shown that the behavior of the concentration is largely influenced by the value of the parameters. The evolution of the concentration may be delayed or accelerated in association with the coupling of the three parameters *β, D* and *R* (Bevilacqua *et al*. 2013).

The third case has no analytical solution. The solution is obtained with the help of the Hermite finite element as shown in the appendix. It is presented the behavior of the solution for the concentration *q(x,y,t)* and the specific flow, both the primary and secondary. In the next chapter, we will present the convergence test for problems in two dimensions. Details on the numerical process may be found in the appendix A.

3.1. Cosine distribution.

Let us assume that the system is homogenous, all parameters $(\beta, D, R)$are constant and the domain of definition is given by $\Omega = [0,1]\times[0,1]$, and $t \geq 0$. Let us consider the problem defined by the set of homogeneous boundary conditions. The boundary conditions correspond to no flux, both primary and secondary. Then $\nabla q(x,y,t)\cdot \vec{n}\Big|_{\partial\Omega} = 0$, $\nabla(\Delta q(x,y,t))\cdot \vec{n}\Big|_{\partial\Omega} = 0$, $(x,y)\in \partial\Omega$. The initial condition is given by:

$$q(x,y,0) = q_0 \cos(2\pi x)\cos(2\pi x)$$

Under these assumptions the solution of the fourth order equation reads:

$$q(x,y,t) = q_0 \exp\left(4\pi^2 D\rho t\right)\cos(2\pi x)\cos(2\pi y),$$

where $\rho = -\beta\left(1+16\pi^2 r(1-\beta)\right)$ with $r=R/D$.

The primary and the secondary fluxes (Bevilacqua *et al*. 2013), corresponding to the particles in the energy states E_1 and E_2, are given respectively by:

$$\mathbf{\Psi}_1 = 2\pi D q_0\left(\sin(2\pi x)\cos(2\pi y)\mathbf{e}_\mathbf{x} + \cos(2\pi x)\sin(2\pi y)\mathbf{e}_\mathbf{y}\right)\exp\left(4\pi^2 D\rho t\right)$$

and

$$\mathbf{\Psi}_2 = 16\pi^3 R\beta q_0\left(\sin(2\pi x)\cos(2\pi y)\mathbf{e}_\mathbf{x} + \cos(2\pi x)\sin(2\pi y)\mathbf{e}_\mathbf{y}\right)\exp\left(4\pi^2 D\rho t\right)$$

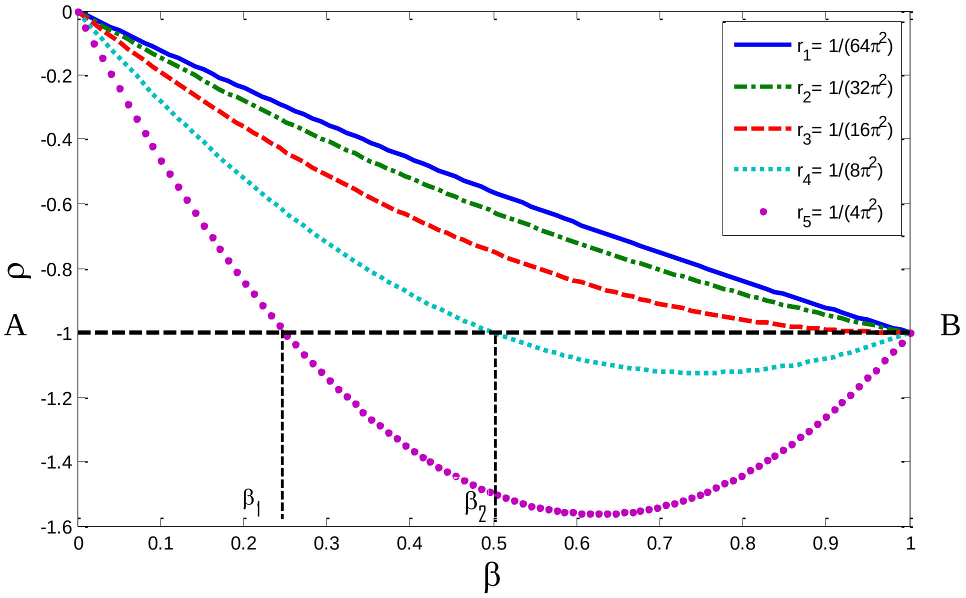


Fig.3.1 Variation of the exponent ρ with the fraction of the diffusing particles β for different values of r corresponding to the density distribution given by $\cos(2\pi x)\cos(2\pi y)$. For pairs (β,r) above $\rho = -1$ the process is delayed characterizing retention as compared with the undisturbed case for β=1

The exponent $\rho = \rho(r,\beta)$ controls the rate of change of the concentration. For $\beta = 1$, the problem is reduced to the classical diffusion problem. The initial distribution fades out with a speed proportional to $-4\pi^2 D$. For other values of β the rate of change of the concentration depends on the ratio r. There is a critical value $r_{crit} = 1/(16\pi^2)$ that defines a separatrix $\rho = \rho(r_{crit},\beta)$ splitting the family of curves into two distinct sets as shown in the Fig.3.1

The separatrix has a minimum at $\beta = 1$. If $r < r_{crit}$ the process is delayed and we may refer to retention because $\rho > -1$ for all values $0 < \beta < 1$. Now, if $r > r_{crit}$ the process is delayed if β falls within an interval $[0, \beta_{crit}]$. The fraction β_{crit} is easily obtained $\beta_{crit} = 1/(16r\pi^2)$. If $\beta > \beta_{crit}$ the exponent ρ falls below –1and the process is accelerated, that is, the particle concentration decays more rapidly as compared to the classical diffusion case.

Consider a certain curve $\rho = \rho(r,\beta)$, $r > r_{crit}$. Since both fluxes **Ψ**$_1$and **Ψ**$_2$travel in the same direction the rarefaction process will be accelerated, that is ρ decreases, provided that the mass flow rate **Ψ**$_2$ is sufficiently large. The mass flow rate of the secondary energy state **Ψ**$_2$ increases with β as seen before. But since the density depends also on the fraction $(1-\beta)$, if this fraction decreases the rarefaction rate varies in the opposite direction and ρ increases. The combination of the accelerating factor β on the mass flow rate and of the slowing factor $(1-\beta)$ avoids the indefinitely decay of $\rho(r,\beta)$. Therefore the exponent $\rho(r,\beta)$reaches a minimum for some value β^* beyond which it starts increasing up to the fixed point –1. The fraction β^* is easily obtained $\beta^* = 1/(32r\pi^2)$.

Clearly, we may refer as delayed only fluxes corresponding to points located above the line AB for which the inequality $\rho > -1$ holds. Substituting the expression for ρ it is immediately obtained $8r\beta\pi^2 < 1$. Now **Ψ**$_2$/**Ψ$_1$ = 8**$r\,\beta\,\pi^2$.Therefore a sufficient condition for the process to be delayed is that **Ψ$_1$>Ψ**$_2$.

In the chapter 4 it will be discussed the interdependence between β and R. All theoretical considerations and solutions of ideal problems lead to the conclusion that the fraction of particles β dispersing according to Fick’s law is an inverse function of R. For very large values of R the fraction β should be small. Therefore the points on the curves with large R corresponding to real cases should be concentrated on the left. Therefore it is plausible to expect that only points to the left of β1 and β2 on Fig. 3.1 correspond to real cases. That is the process for the initial and boundary conditions exposed in this case is delayed as compared with the Fick’s diffusion

3.2. Hyperbolic cosine distribution.

Let us consider now another particular system where all parameters $(\beta, D, R)$are constant, the domain of definition is given by$[0,1]\times[0,1]$ and $t \geq 0$, and the new set of boundary conditions reads: $q(x,y,t)=0.5a^2\nabla^2 q(x,y,t)$,$\nabla q(x,y,t)=0.5a^2\nabla^3 q(x,y,t)$ Together with the initial condition:

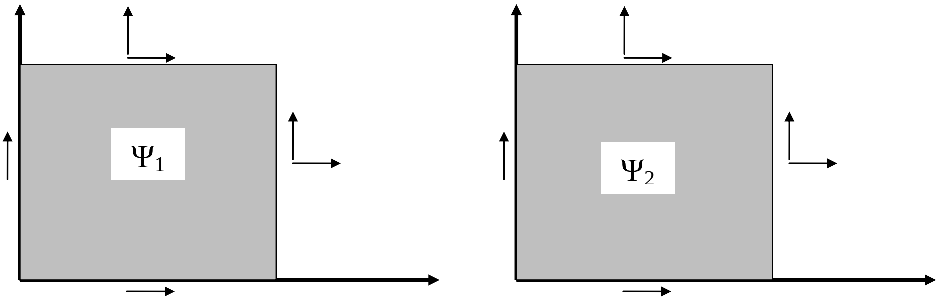


Fig.3.2 The two fluxes on the boundary

$$q(x,y,0)=q_0\cosh\left(\frac{x}{a}\right)\cosh\left(\frac{y}{a}\right)$$

Under these assumptions the solution of the fourth order equation reads:

$$q(x,y,t)=q_0\exp\left(\frac{2D}{a^2}\rho t\right)\cosh\left(\frac{x}{a}\right)\cosh\left(\frac{y}{a}\right)$$

where $\rho=\beta\left(1-\frac{2r}{a^2}(1-\beta)\right)$. The primary and secondary fluxes (Bevilacqua *et al*. 2013), corresponding to the particles in the energy states E_1 and E_2 are given respectively by:

$$\boldsymbol{\Psi}_1=-q_0\frac{D}{a}\left(\sinh\left(\frac{x}{a}\right)\cosh\left(\frac{y}{a}\right)\mathbf{e_x}+\cosh\left(\frac{x}{a}\right)\sinh\left(\frac{y}{a}\right)\mathbf{e_y}\right)\exp\left(\frac{2D}{a^2}\rho t\right)$$

And

$$\mathbf{\Psi}_2 = q_0 \frac{2R}{a^3}\beta\left(\sinh\left(\frac{x}{a}\right)\cosh\left(\frac{y}{a}\right)\mathbf{e}_{\mathbf{x}} + \cosh\left(\frac{x}{a}\right)\sinh\left(\frac{y}{a}\right)\mathbf{e}_{\mathbf{y}}\right)\exp\left(\frac{2D}{a^2}\rho t\right)$$

This case represents, in principle, a densification process. That is, it is expected that the concentration tends to increase in time as the particles belonging to the primary flux feed the supporting medium through the side $x = 1,\ 0 \le y \le 1$ and $y = 1,\ \ 0 \le x \le 1$ of the border. If there is no disturbance in the diffusion process, $\beta = 1$, the rate of change of density is equal to $2D/a^2$. Fig.2.3 shows the variation of ρ with β for different values of r/a^2 . As in the previous case there is a critical value of r/a^2 namely $\left(r/a^2\right)_{crit} = 0.5$, defining a separatrix $\rho_{crit}(\beta) = \rho\left(\beta, \left(r/a^2\right)_{crit}\right)$, such that if $r/a^2 < \left(r/a^2\right)_{crit}$ the concentration tends to grow continuously, although slowly as compared with the case $\beta = 1$, characterizing a densification process irrespectively of the fraction β of particles. Now for $r/a^2 > \left(r/a^2\right)_{crit}$ there is a maximum value of the fraction of the diffusing mass that we call β_{crit} given by $\beta_{crit} = 1 - a^2/r$ such that for all $\beta < \beta_{crit}$ the density tends to decrease, following a rarefaction process. That is, for branches below the axis $\rho = 0$ the process is reversed, instead of densification, rarefaction prevails. The mass of particles leaving the system overcomes the mass of the incoming particles inducing an overall decrease in the particle concentration.

It is remarkable that for particular combinations $\left(r/a^2, \beta_{crit}\right)$ such that $\rho\left(r/a^2, \beta_{crit}\right) = 0$ the concentration is kept constant in time in spite of the fact that the

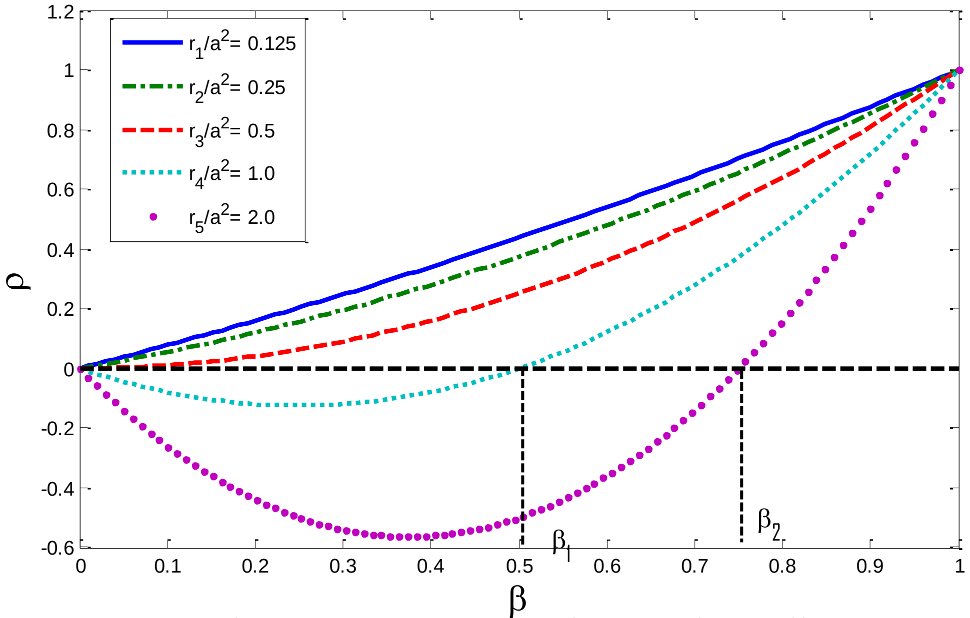


Fig.3.3 Variation of the exponent ρ with the fraction of the diffusing particles β in the energy state for different values of the r corresponding to the density distribution given by $\cosh(x/a)\cosh(y/a)$. For pairs (β,a^{2}r) below AB the process is delayed characterizing retention as compared with the undisturbed case $\beta = 1$.

system continues to be dynamically active. The critical points on the β axis will be called stagnation points. If $\beta > \beta_{crit}$ the density increases steadily but if $\beta < \beta_{crit}$ the concentration $q(x,t)$ tends to fade out. As stated previously the conversion of densification into rarefaction is controlled by the mass flow rate $\mathbf{\Psi}_2$ and the corresponding particle fraction $(1-\beta)$.

As shown in the previous examples the solution of the fourth order equation with prescribed boundary conditions may lead to delay or acceleration in the diffusion process, despite the fact that the discrete approach assumed retention in the redistribution rule. The mass conservation principle however doesn't impose any restriction concerning the type of evolution. For the continuum approach it is enough to prescribe the corresponding flux laws. Therefore we may expect both, delay or acceleration depending on the initial and boundary conditions.

As in the previous example considering the fraction β as a decreasing function of time it is reasonable to admit that for large values of R the real solution will be displaced to the left where β is small. Therefore for the case of primary and secondary fluxes in opposite directions the tendency when R is large is to cause a rarefaction process opposing the tendency of the classical theory.

3.3. Particular pulse functions as initial condition

In this section, we present some numerical solutions in 1D and 2D for particular types of initial conditions that may induce a fluctuation profile of the concentration distribution and consequently a sequence of maxima and minima of the concentration profile. The mathematical analysis concerning extreme values of the solution of fourth order partial differential equations has not yet lead to definite answers. The numerical solution presented in the sequel for a particular initial condition may indicate interesting hints for the future mathematical analysis. Even if there are no formal proofs for some of the mathematical properties of the numerical solution the restrictions imposed on the initial condition may suggest new investigation lines. It will also be shown the long run behavior of some particular solutions. For some cases the initial acceleration process may reverse to a delayed behavior compared with the classical solution.

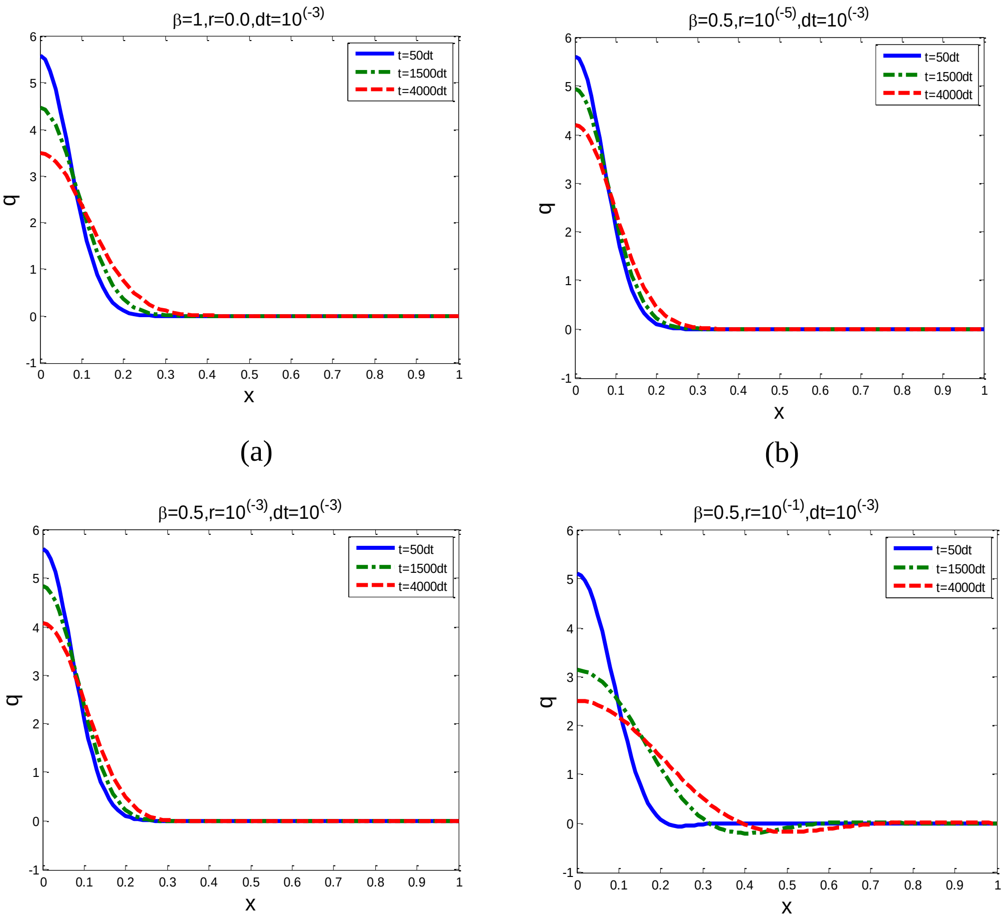
Let us initially consider the normal distribution defined in the interval [0,1] (Bevilacqua *et al*. 2013):

$$q(x,0) = \frac{1}{\sqrt{\pi\theta^2}} \exp\left(-\frac{x^2}{\theta^2}\right)$$

Let θ=0.1. The boundary conditions prescribe no flux at both extremities of the interval that is $\boldsymbol{\Psi}_1$=0 and $\boldsymbol{\Psi}_2$=0, which means that the first and third derivatives vanish fo x=0 and x=1. This is a pulse at the origin. Let us examine the solution of the bi-flux equation for r=10^{-5} , r=10^{-3} and r=10^{-1} where r=R/D.

The solution was obtained with the Hermite finite element for integration in space and Newton backward difference method for time integration (Reddy, 1993; Young and Hyochoong, 1997). All the results presented in this chapter were obtained with the same method. The details are presented on the appendix A, together with the convergence tests.

The evolution of the concentration in the interval $[0,1]$ is shown in Fig.3.4 for $\beta = 0.5$ and three different values of r, Fig.3.4 (b),(c),(d). It is also displayed the solution for the classical Fick´s diffusion process, Fig.3.4 (a). Note that β=0.5 gives the maximum value for β(β−1) and therefore for this value of β it is expected the maximum



(a) (b)

(c) (d)

Fig.3.4. Evolution of the concentration profiles for different values of the reactivity coefficient *R* controlling and the fraction of particle in the primary flux: (a): $\beta = 1$ $R = 0.0$ (b): $\beta = 1.0$, $\beta = 0.5$ (c): $r = 10^{-5}$, $\beta = 0.5$ (d): $r = 10^{-3}$, $\beta = 0.5$ *dt* is the time interval.

perturbation on the classical solution imposed by the fourth order term for a fixed R. For very small values of the ratio $r=10^{-3}$ and $r=10^{-5}$ there is clearly a delay in the process that can be seen by comparing figures 3.4(a) with 3.5(b) and 3.5(c). Indeed for the time (4000dt), the concentration at x=0 according to the classical solution is of the order q_0 = 3.5 units and for $r=10^{-5}$ and $r=10^{-3}$ are q_0 = 4.2 units and q_0 = 4.08 respectively.

However for $r=10^{-1}$ the process is initially accelerated as can be seen from Fig.3.4(d) with the concentration at x=0 for t=4000dt going down to a value close to $q_0 = 2.5$.

It was noticed from several tests that solutions with initially speeding processes display consistently at least one minimum in the interval $[0,1]$ as shown in Fig.3.4 (d) with $r=10^{-1}$. For these cases the concentration becomes negative for some subinterval $[x_1, x_2] \subset [0,1]$. This behavior has already been reported for fourth order parabolic equations (Murray, 2008; Cohen *et al.* 1981)

Deviating from this peculiar characteristic, for a particular range of the parameters r the solution may follow the regular physically compatible variation, that

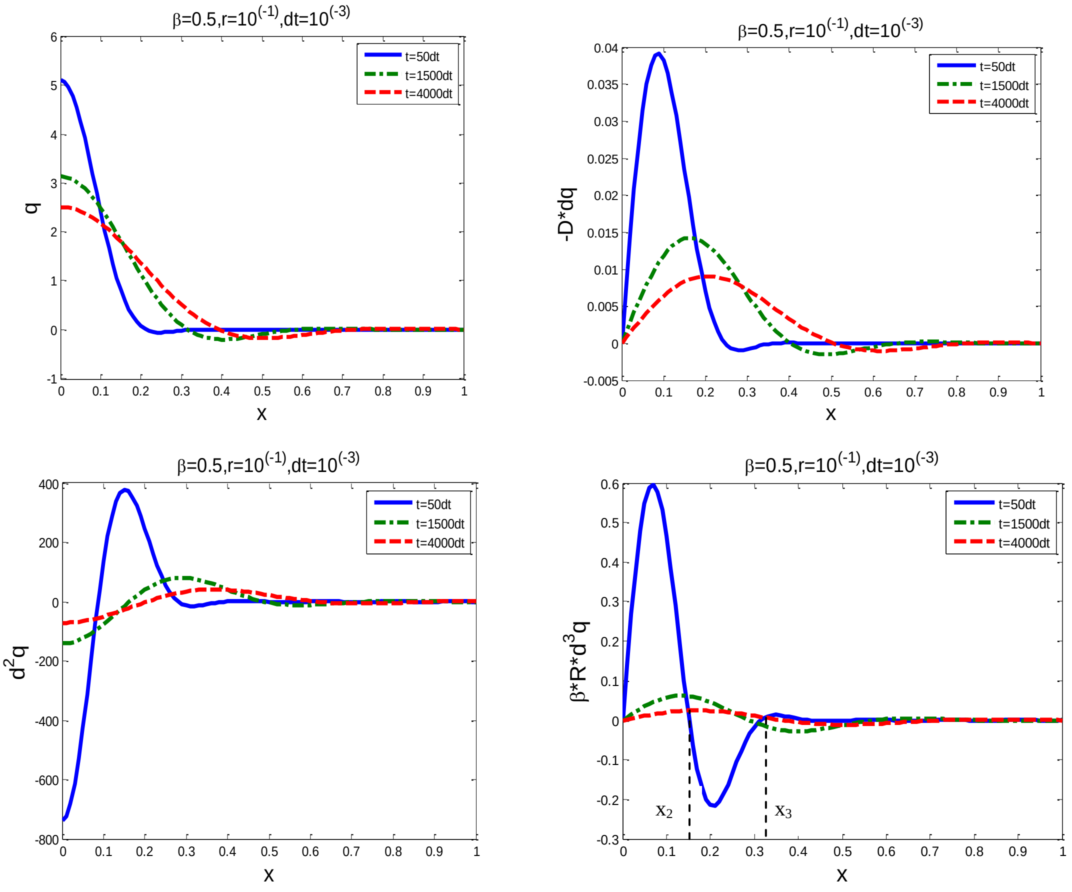


Fig.3.5. Evolution of the concentration , the first flux, the curvature , the second flux with $D = 0.001$, $\beta = 0.5$, $r = 10^{-1}$.

is, no extreme in $[0,1]$ except for $x=0$ and $q(x,\mathrm{t})>0$ for $t>0$ and $0\leq x\leq 1$. Indeed for all cases of high values of the retention coefficient with a fixed diffusion coefficient, that is r small, $r=10^{-3}$ and $r=10^{-5}$, the numerical solution doesn't induce any observable anomaly and the concentration remains positive for all time in $[0,1]$. If this is not a demonstration, since we are dealing with numerical solutions the indication is sufficiently strong to support the conjecture that $q(x,\mathrm{t})>0$ in the space domain for all time provided that r is sufficiently small.

Negative values of the concentration may occur for certain combinations of r and β as shown above. This phenomenon has a physical meaning. For the initial condition introduced above the primary and the secondary fluxes travel in the positive x-axis direction close to the origin, that is for $x<x_1$. The secondary flux changes sign at a point x_2 and keeps forcing particles to move in the negative direction of the x-axis in given interval $[x_2, x_3]$. For certain values of r and β even the primary flux changes sign in an interval that coincides partially with $[x_2, x_3]$. This means that in a region close to the origin a counter flux appears recruiting particles from the right to the left as shown in Fig.3.4. If the intensity of the counter flux is strong enough it is possible that the stock of particles will be not able to supply the demand created by this inversion of motion. In these cases the concentration becomes negative.

Now if the reversed secondary flux intensity is moderate the primary flux remains always positive along the x-axis and the concentration will not drop below zero. This case corresponds to a standing retention behavior, that is, the process is delayed for all time. Negative values of the concentration are always associated, for the type of initial and boundary conditions assumed here, with processes which are initially subjected to acceleration. Therefore when the decaying speed of the concentration exceeds the value corresponding to the classical diffusion the solution is physically compatible only if there is an initial layer that can supply particles for some bounded interval in the domain $[0,1]$ otherwise the model is not valid anymore and the concentration continuity will be disrupted causing strong instability in the process.

Now if we consider the variation in time of the concentration at the origin, $x=0$, for a fixed $\beta=0.5$, $D=0.007$ and different values of r the results obtained for the case of initial and boundary conditions as prescribed above show that the processes that are initially accelerated may become delayed with respect to the classical diffusion approach after a sufficiently long time. With $r=10^{-1}$, for instance, the process is initially accelerated as compared with the classical case $R=0$ and $\beta=1.0$ as shown in Fig.3.6. But for $t=10$ the solution is reversed, the concentration for $r=10^{-1}$ is larger than the corresponding value for the case of classical diffusion. So in the long run we may say that the process is delayed.

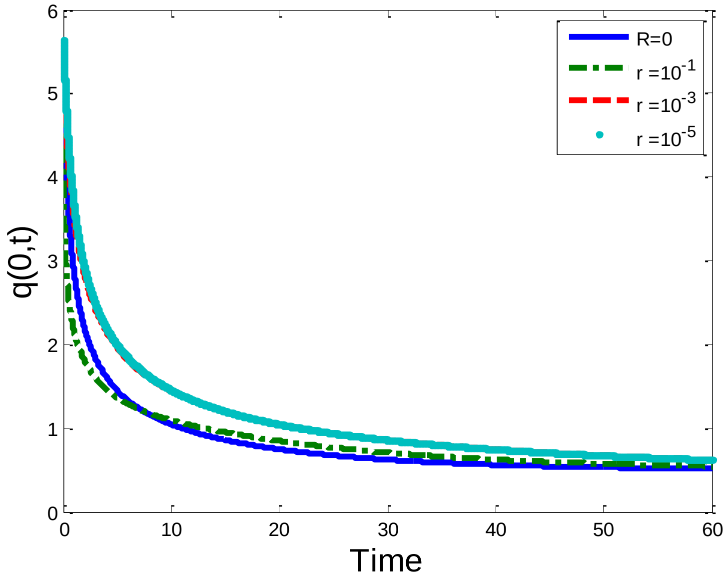


Fig. 3.6.Evolution of the concentration at $x=0$ for different values of the reactivity coefficient R. the blue line represents the classical diffusion with $R=0$ and $\beta=1$

The behavior of the secondary flux is crucial regarding the evolution of the concentration since the third order derivative depends on the intensity and on the sign of that function. Now the secondary flux represents the curvature variation of the concentration profile. This is another important aspect of the initial condition equivalent to the gradient variation. As the concentration varies in time the sign of the second flux and the primary flux as well may switch from positive to negative, or the other way around, inducing reversal of the flow direction. The solution therefore turns out to be much more complex than for the classical diffusion equation.

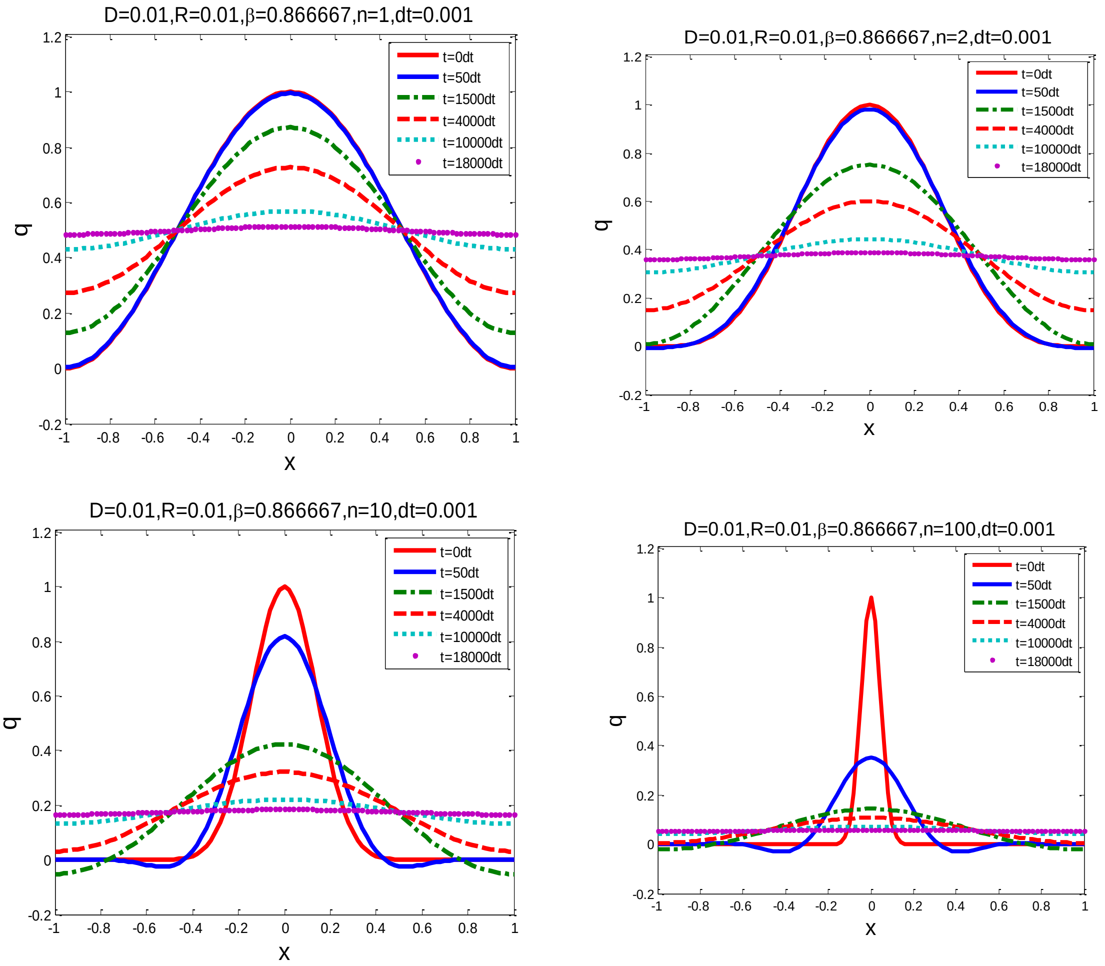
In order to explore the conditions that triggers fluctuations in the concentration profile, let us examine the solutions for a particular form of initial conditions. Consider the bi-flux equation with all coefficients constant:

$$\frac{\partial q(x,t)}{\partial t}=\frac{\partial}{\partial x}\left[\beta D\frac{\partial q(x,t)}{\partial x}\right]-\frac{\partial}{\partial x}\left[\beta(1-\beta)R\frac{\partial^3 q(x,t)}{\partial x^3}\right]$$

defined in the interval[–1,1].

Let the initial condition be given by: $q(x,0)=(0.5(1+\cos(\pi x)))^n$ and the boundary condition by: $\partial q(-1,t)/\partial x=0$, $\partial q(1,t)/\partial x=0$, $\partial^3 q(-1,t)/\partial x^3=0$ $\partial^3 q(1,t)/\partial x^3=0$. In the previous examples the initial condition was kept constant while the solution was obtained for three different values of r=R/D to see how this parameter influence the evolution of the concentration profile with possible occurrence of fluctuations. In the present case the initial condition plays the key role since it is modified increasing the value of n such that it approaches gradually a pulse at the origin. It is a peculiar type of pulse that approaches a Dirac function as n→∞. In any case it provides very interesting information about the evolution of the solution and the induction of fluctuations behavior. We take r=R/D=1 and β=0.86667. Note that this value of β ia equivalent to take β=0.13333 as far as the influence of the fourth order term is concerned keeping th same R. The difference of the solutions will be determined by the coefficient of the second order term βD. The primary flux is not affected by the value of β but the secondary flux depends linearly on this parameter. Therefore for the examples presented here $\mathbf{\Psi_2}$ is maximized with respect to β.

Let us examine the solution for some values of n. Note that the initial condition remains less than one for all points of the interval, except for x=0, since (1+cos(πx))/2<1 for all $-1 \le x < \varepsilon$ and 1 $\varepsilon < x \le 1$. The initial condition is progressively being concentrated at x=0 for increasing values of n. For n=1 clearly all the concentration profile remains positive. The same is valid for n=2. For increasing values of n however the solution degenerates and for n=10 the concentration profile presents fluctuations with negative values for certain time intervals. For sufficiently large time the solution becomes again regular and tends to a uniform distribution as expected since there are no fluxes at the boundaries.



D=0.01,R=0.01,β=0.866667,n=1,dt=0.001

D=0.01,R=0.01,β=0.866667,n=2,dt=0.001

D=0.01,R=0.01,β=0.866667,n=10,dt=0.001

D=0.01,R=0.01,β=0.866667,n=100,dt=0.001

Fig.3.7 The numerical solution for the fourth condition equation with no flux boundary condition

Let us now test another type of boundary condition letting the flux free at both extremities of the interval and imposing the concentration and the concentration curvature to vanish at x=1 an x=−1. That is $q(-1,t)=0$, $q(1,t)=0$, $\partial^2 q(-1,t)/\partial x^2 = 0$, $\partial^2 q(1,t)/\partial x^2 = 0$. The initial condition is $q(x,0)=\cos^n(0.5\pi x)$.The parameters R,D and β are the same as before.

The solutions present the same general behavior as in the previous case except that now the solution remains without fluctuation for higher values of n, Fig.3.8. For n=10 for instance the solution for this case, that is free flux at the boundaries, is regular $q(x,t) \geq 0$ for all $1 \geq x \geq -1$. For the previous case with no flux at the boundaries the anomaly, $q(x,t) < 0$ is present for a subset of the domain of definition. For n=100 however the anomalous behavior shows up.

Therefore it is possible to say that the occurrence of anomalies, fluctuations in this case, depends on the boundary conditions at least for some class of functions.

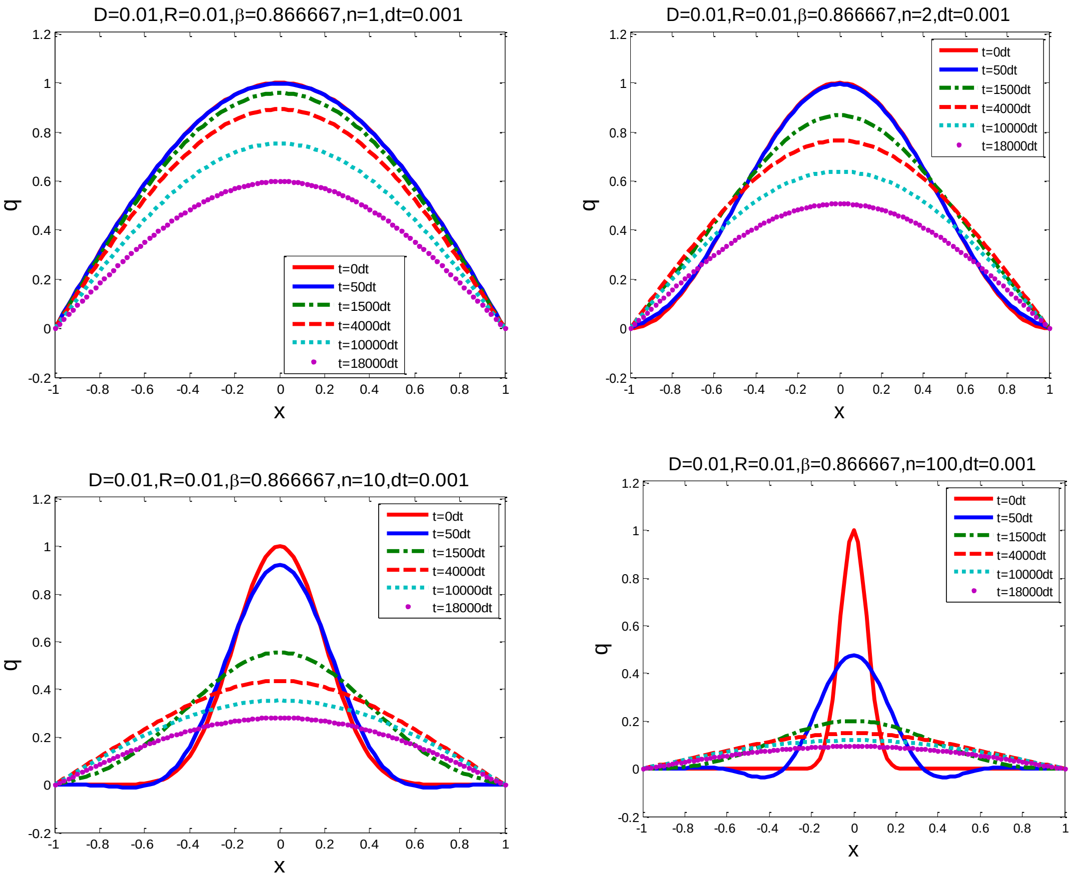


Fig.3.8 The numerical solution for the fourth condition equation with Dirichlet and Navier boundary condition

These examples show that there must be a limiting condition, or a definite critical initial condition that we may call separatrix characterizing two different behaviors, the regular behavior and the anomalous behavior with presence of fluctuation and negative values of the concentration. These indications can well be used to start theoretical analysis of the behavior of fourth order partial differential equations.

To close this chapter let us consider a 2-D problem defined in the region $[-1,1]x[-1,1]$. The problem is to solve the bi-flux equation:

$$\frac{\partial q}{\partial t} = \nabla \cdot (\beta D \nabla q) - \nabla \cdot (R\beta(1-\beta)\nabla(\Delta q))$$

with all parameters constant, namely $\beta = 0.5$, $D = 0.01$, $R = 0.38$. The boundary conditions correspond to no flux at the boundaries:

$$\mathbf{\Psi}_1\big|_{x=\pm 1} = 0 \qquad \mathbf{\Psi}_1\big|_{y=\pm 1} = 0 \qquad \mathbf{\Psi}_2\big|_{x=\pm 1} = 0 \qquad \mathbf{\Psi}_2\big|_{y=\pm 1} = 0$$

and the initial condition is given by:

$$q(x, y, 0) = e^{-10\left(x^2 + y^2\right)}$$

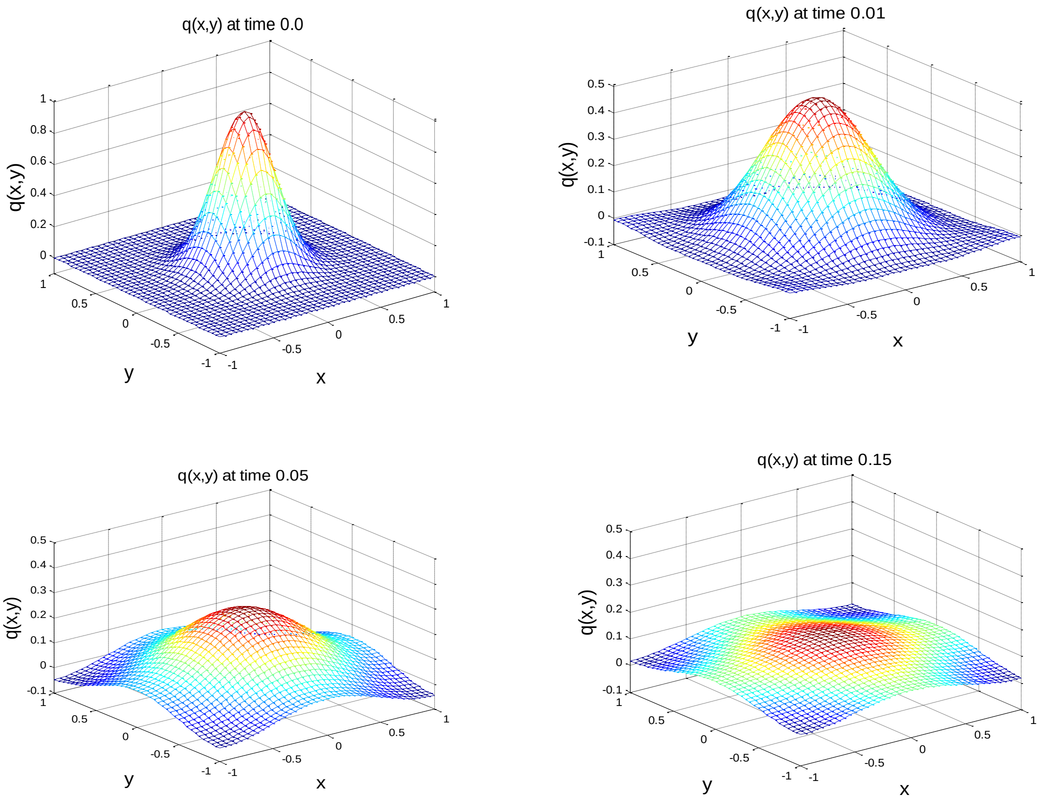


Fig.3.9. The behavior of concentration at t=0.0; 0.01; 0.05; 0.15

Fig.3.9 shows the concentration distribution at different times. It is interesting to see that as time pass by the particles moving towards the edges tend to concentrate at the center of the middle of the edges, x=0, y=±1 and y=0, x=±1. Particles reach the central part of the edge before reaching the corners. This can be explained by the fact that the central part of the edge is closer to the initial distribution of particles, that is, the initial conditions. Initially the anomalous behavior corresponding to negative values of the concentration is present at the corners Fig.3.9. Due to the high gradient from the center to the corners the flux is oriented towards the corners inducing a fourfold partition. The density and flux distribution are similar in the four quadrants. In relatively short time four wells grow at the corners inducing the fluxes to converge to these four points. Fig.3.10 to Fig. 3.12 shows clearly this behavior.

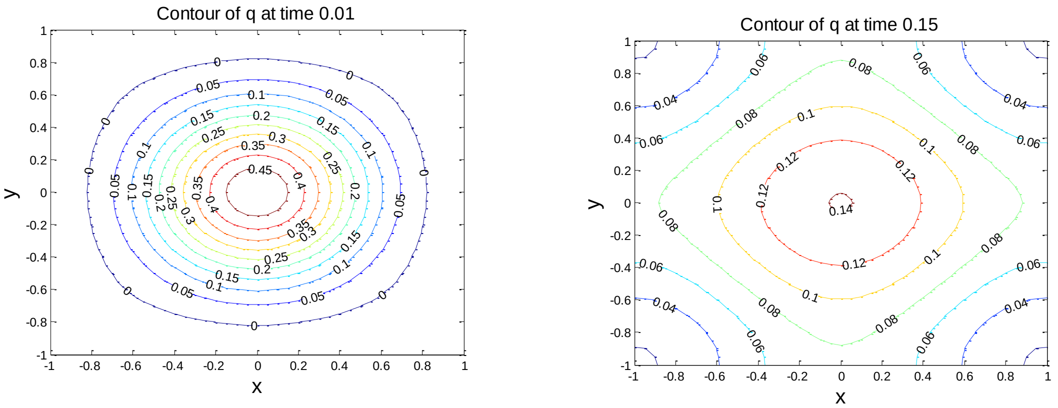


Fig.3.10. The contour of the concentration at time 0.01 and 0.15

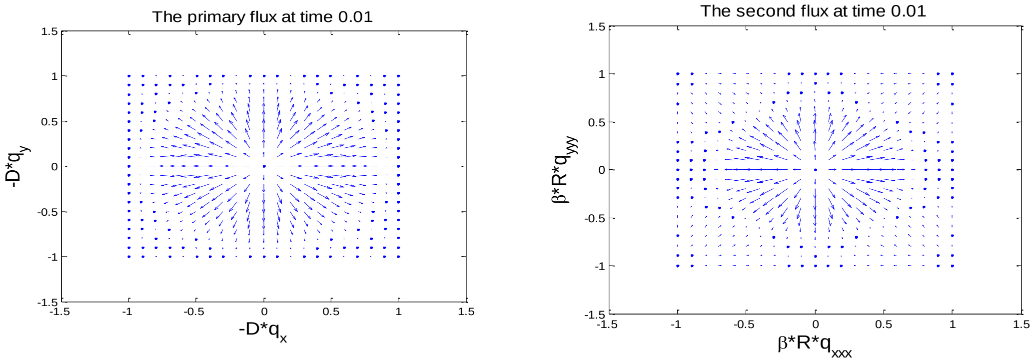


Fig.3.11. The primary and the second flux at time 0.01

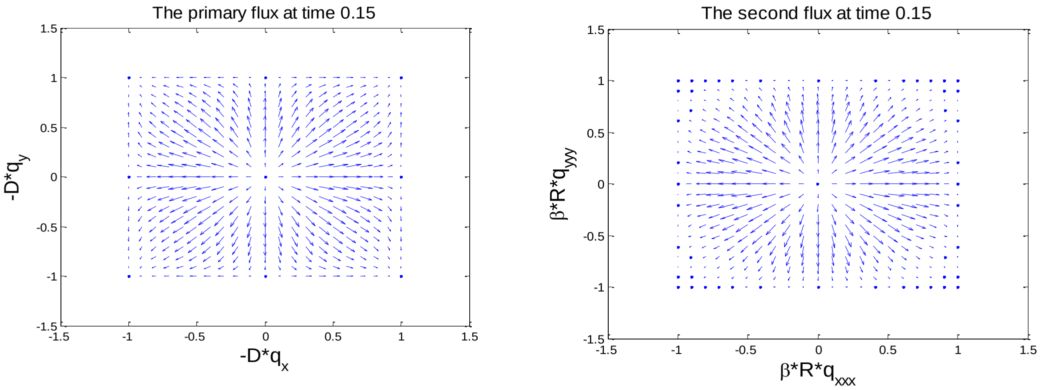
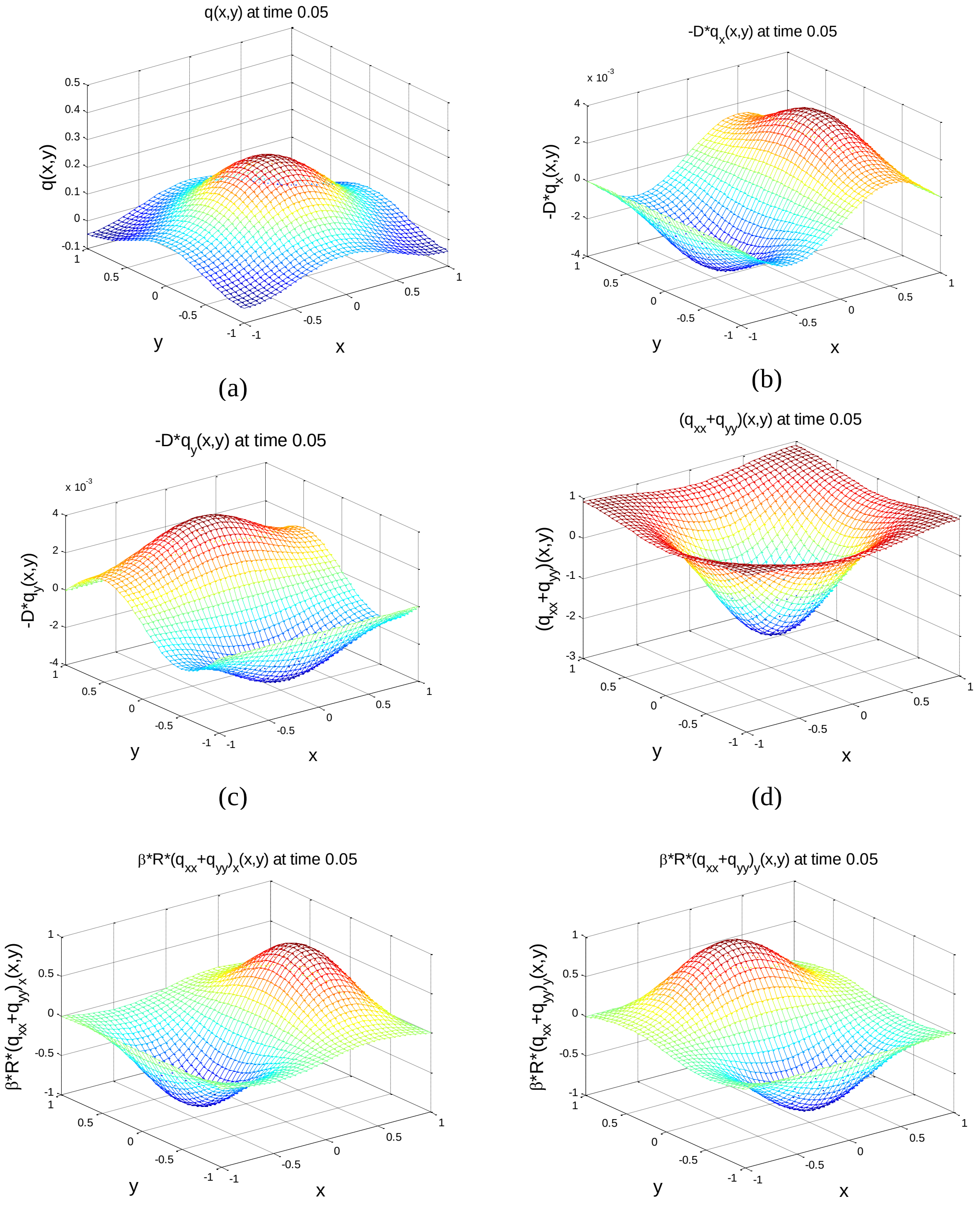


Fig.3.12. The primary and the second flux at time 0.15

Fig.3.13a show the density distribution on the domain [−1,1]x[−1,1] for t=0.05 and Fig.3.13d the curvature of that same distribution. The other figures show the distributions of the effective primary flux and the effective secondary flux which are the correlated with the gradients of the density and curvature distribution respectively.



(a) (b)

(c) (d)

(e) (f)

Fig.3.13. the behavior of the concentration and the primary and the second flux at time 0.05

The general behavior of the solution for the classical Fick’s diffusion process follows similar evolution process, except that there are no singularities at the corners. The distribution remains positive for points of the domain all the time.

We will see that this expected behavior for the diffusion process may be completely different for the case of anisotropic media.

Chapter 4

Anisotropic diffusion processes 1D case

In the previous chapters it was presented the bi-flux process for isotropic media. Some basic differences in the behavior of this new approach as compared with the Fick´s diffusion were highlighted. It was shown that there are critical combinations for the pair (β_{crit},R_{crit}) dividing the concentration evolution into two different zones. One of them exciting delaying processes while the other induces acceleration, or one region corresponding to accumulation while for the other rarefaction prevails. The combination of these two parameters is therefore critical for the anomaly introduced in diffusion process.

The correlation between β and R was carefully examined by Silva, *et al.* (2013 and 2014), Faria, *et al.* (2015). After the simulation of inverse problems for the bi-flux equation it was clearly shown that there is a correlation between these two parameters. This correlation is not surprising. The secondary flux excited by the presence of the reactivity coefficient R automatically captures a fraction β of particles for this new energy state.

There is no definite relationship between these new parameters. It is a new challenge of this theory together with, at least, another critical point that we will see later. The only clue for helping the definition of β as function of R, β=F(R) is that it is a decreasing function of R and for R=0, β=1. Two laws will be used to solve some typical problems, namely:

a) A linear law of the form:

$\beta = 1 - \gamma\left(\dfrac{R}{R_{\max}}\right)$ where $0 \le R \le R_{\max}$ and $0 \le \gamma \le 1$ is a saturation parameter that is β cannot be less than 0.

b) An exponential law of the form:

$$\beta = \exp\left(-\alpha \left(\frac{R}{R_0} \right)^2 \right) \quad \text{where } R \geq 0 \text{ and } \alpha \geq 0$$

There are of course several other possibilities, but as far as we know, there is no concrete justification to adopt a definite rule to connect these two parameters. Probably there is no unique law. It will depend on the substratum and on the nature of the spreading particles. As for the determination of the existence and properties of the complex flux behavior exposed in this thesis, experimental data are not yet available.

A second critical question is the definition of the secondary flux. For the case of isotropic media the secondary flux is well defined, that is, it is uniquely defined:

$$\mathbf{\Psi}_2^1 = R\beta \frac{\partial^3 q(x,t)}{\partial x^3} \mathbf{e}_x$$

Now if β and R are function of x there are other possible definitions for the secondary flux, as already mentioned. Recall the other two possibilities:

$$\mathbf{\Psi}_2^2 = R \frac{\partial}{\partial x} \left(\beta \frac{\partial^2 q(x,t)}{\partial x^2} \right) \mathbf{e}_x$$

and

$$\mathbf{\Psi}_2^3 = R \frac{\partial^2}{\partial x^2} \left(\beta \frac{\partial q(x,t)}{\partial x} \right) \mathbf{e}_x$$

We will call these three expressions as first class, second class and third class secondary fluxes respectively. Each of these definitions leads to a particular governing equation.

For $\mathbf{\Psi}_2^1$:

$$\frac{\partial q}{\partial t} = \left[\frac{\partial(\beta D)}{\partial x} \right] \frac{\partial q}{\partial x} + [\beta D] \frac{\partial^2 q}{\partial x^2} - \left[\beta \frac{\partial(R(1-\beta))}{\partial x} + R(1-\beta) \frac{\partial \beta}{\partial x} \right] \frac{\partial^3 q}{\partial x^3} - R(1-\beta)\beta \frac{\partial^4 q}{\partial x^4} \quad (4.1)$$

For $\mathbf{\Psi}_2^2$:

$$\begin{aligned} \frac{\partial q}{\partial t} &= \left[\frac{\partial(\beta D)}{\partial x} \right] \frac{\partial q}{\partial x} + \left[\beta D - \frac{\partial(R(1-\beta))}{\partial x} \frac{\partial \beta}{\partial x} - R(1-\beta) \frac{\partial^2 \beta}{\partial x^2} \right] \frac{\partial^2 q}{\partial x^2} - \\ &- \left[\beta \frac{\partial(R(1-\beta))}{\partial x} + 2R(1-\beta) \frac{\partial \beta}{\partial x} \right] \frac{\partial^3 q}{\partial x^3} - R(1-\beta)\beta \frac{\partial^4 q}{\partial x^4} \end{aligned} \quad (4.2)$$

For $\mathbf{\Psi}_2^3$:

$$\frac{\partial q}{\partial t} = \left[\frac{\partial(\beta D)}{\partial x} - \frac{\partial}{\partial x}\left(R(1-\beta)\frac{\partial^2 \beta}{\partial x^2} \right) \right] \frac{\partial q}{\partial x} + \left[\beta D - 2\frac{\partial(R(1-\beta))}{\partial x}\frac{\partial \beta}{\partial x} - 3R(1-\beta)\frac{\partial^2 \beta}{\partial x^2} \right] \frac{\partial^2 q}{\partial x^2}$$
$$- \left[\beta \frac{\partial(R(1-\beta))}{\partial x} + 3R(1-\beta)\frac{\partial \beta}{\partial x} \right] \frac{\partial^3 q}{\partial x^3} - R(1-\beta)\beta \frac{\partial^4 q}{\partial x^4} \tag{4.3}$$

These three equations clearly present considerable differences in the factors of the concentration derivatives. This is of crucial importance. Indeed, the equation corresponding to the secondary flux given by $\mathbf{\Psi}_2^1$ is similar to the classical equation for anisotropic media. It is the same with the diffusion coefficient modified to βD. If D is constant the bi-flux equation with this definition for the secondary flux introduces an artificial anisotropy for the primary flux. The reactivity coefficient doesn't play any direct role in the classical diffusion process. The perturbation introduced by R is indirect through the partition coefficient β.

Now the second and third definitions of $\mathbf{\Psi}_2$ involves considerable perturbation in the primary flux even if the diffusion coefficient D is constant. This means that for these cases the constants associated to the secondary flux are mingled to the constants of the primary flux. The perturbation imputed by the secondary flux in the primary flux is of considerably importance.

By the time being there is no definite reason to decide for one of the three. Certainly the first definition $\mathbf{\Psi}_2^1$ is the less critical, that is, it will probably introduce less serious disturbances in the solution, while the other two $\mathbf{\Psi}_2^2$ and $\mathbf{\Psi}_2^3$ may input essential differences in the flux as functions of space and time. If we assume that every potential is generated by the gradient of some appropriated field, the second option $\mathbf{\Psi}_2^2$ is the more appropriate. Indeed R is the characteristic constant and the field is given by the concentration curvature $1/r \propto \partial^2 q/\partial x^2$ weighted by the fraction β of diffusing particles. Than the second proposal matches these conditions. Therefore there are strong reasons to consider $\mathbf{\Psi}_2^2$ the best option.

Finally, it is possible to have also the physical constants varying with time for isotropic or anisotropic diffusion. In general this condition doesn't introduce any major difficulty in the solution.

It must be clear that we have found no references on bi-flux diffusion further than those already cited. Therefore the solutions that will be presented in the sequel are in fact, numerical experiments that try to analyze the influence of the new physical constants on the concentration distribution. Comparisons with the classical model will be included for some cases. The solutions will also be associated to some particular phenomenon that supposedly could be model with the theory under discussion.

4.1Diffusion processes in an anisotropic one-dimensional medium

Consider the interval $[-1,1]$ and an anisotropic substratum referred to the secondary flux parameters only. That is D=0.01 and $R(x) = R_0 \exp(-20(x-0.5)^2)$, $R_0 = 0.5$ Initial condition: $q(x,0) = 0.25(1+\cos(\pi x))$, and boundary condition:

$$\partial q(-1,t)/\partial x = 0,\ \partial q(1,t)/\partial x = 0,\ \partial^3 q(-1,t)/\partial x^3 = 0, \partial^3 q(1,t)/\partial x^3 = 0$$

Let us assume the correlation between R and β given by the linear law:

$$\beta = 1 - 2R/3R_0$$

The secondary flux will be defined as the first proposal $\mathbf{\Psi}^1_2$. This choice minimizes the perturbation of the anisotropy on the solution, and therefore gives the opportunity to verify the minimum deviation from the classical one. That is,

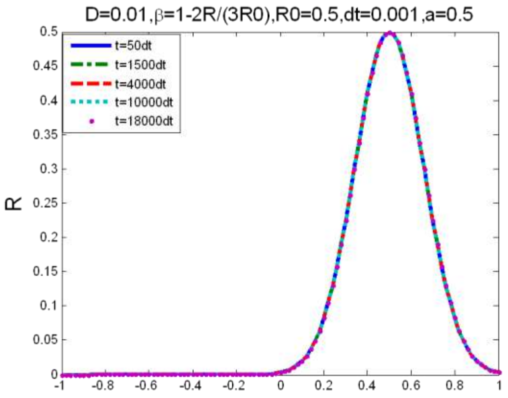


Fig. 4.1 Initial distribution *R*

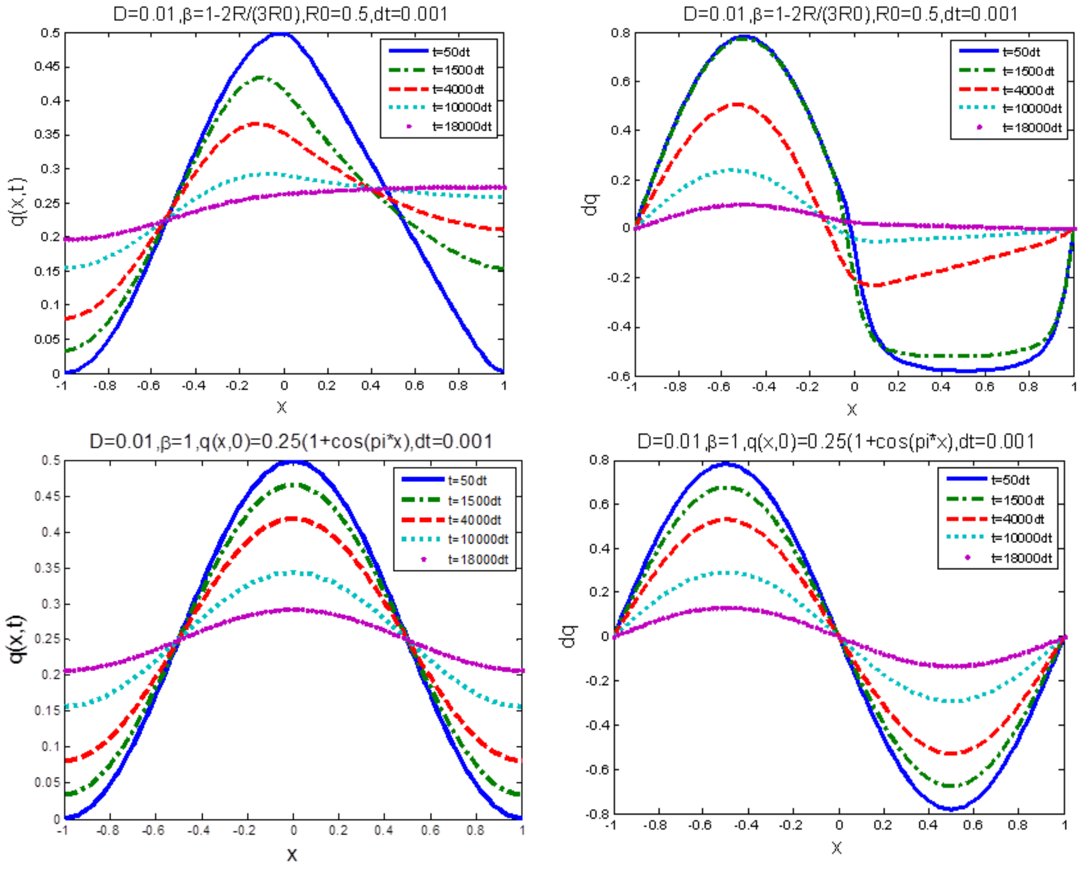


Fig.4.2 Evolution of q and first derivative comparing the classical medel

this is what the theoretical development has induced up to now.

The equation to be solved is therefore:

$$\frac{\partial q(x,t)}{\partial t}=\frac{\partial}{\partial x}\left[\beta D\frac{\partial q(x,t)}{\partial x}\right]-\frac{\partial}{\partial x}\left[\beta(1-\beta)R\frac{\partial^3 q(x,t)}{\partial x^3}\right]$$

with the definitions given above. Note that the reactivity coefficient varies as shown in the Fig.4.1 The medium is isotropic on the first half and the anisotropy assigned by the variation of R occurs on the second half with a maximum at x=0.5.

Fig.4.2 shows the solutions for the bi-flux process and the classical Fick´s method. Both the concentration and the specific primary flux ($\boldsymbol{\Psi}_{1(spec)}=\partial q/\partial x$) are shown. There is clear tendency for the concentration to become denser on the right half of the interval where R is large. As t→∞ the concentration tends to a uniform distribution for both cases as it should be. It is also clear that the primary flux, for the bi-flux diffusion Fig.4.2b, keeps the maximum intensity $\boldsymbol{\Psi}_{1(spec)}\approx 0.6$ along all the points on the half x>0.5. The primary flux distribution for the classical case Fig.4.2d despite presenting a higher maximum values $\boldsymbol{\Psi}_{1(spec)}\approx 0.8$ at x=0.5 doesn't sustain this intensity for a large interval. Also the secondary flux, Fig.4.3, pushes the particles towards the end x=1with two intense bursts close to x=0 and x=1.

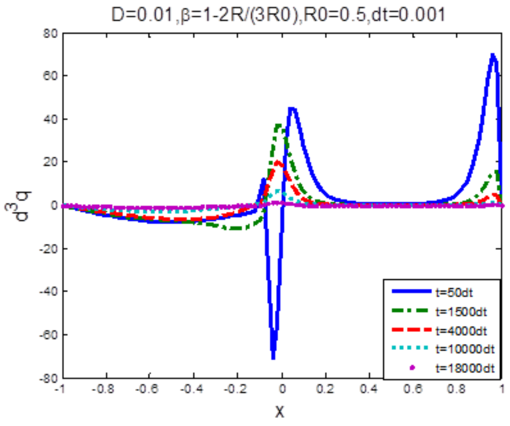


Fig.4.3 The behavior of second flux

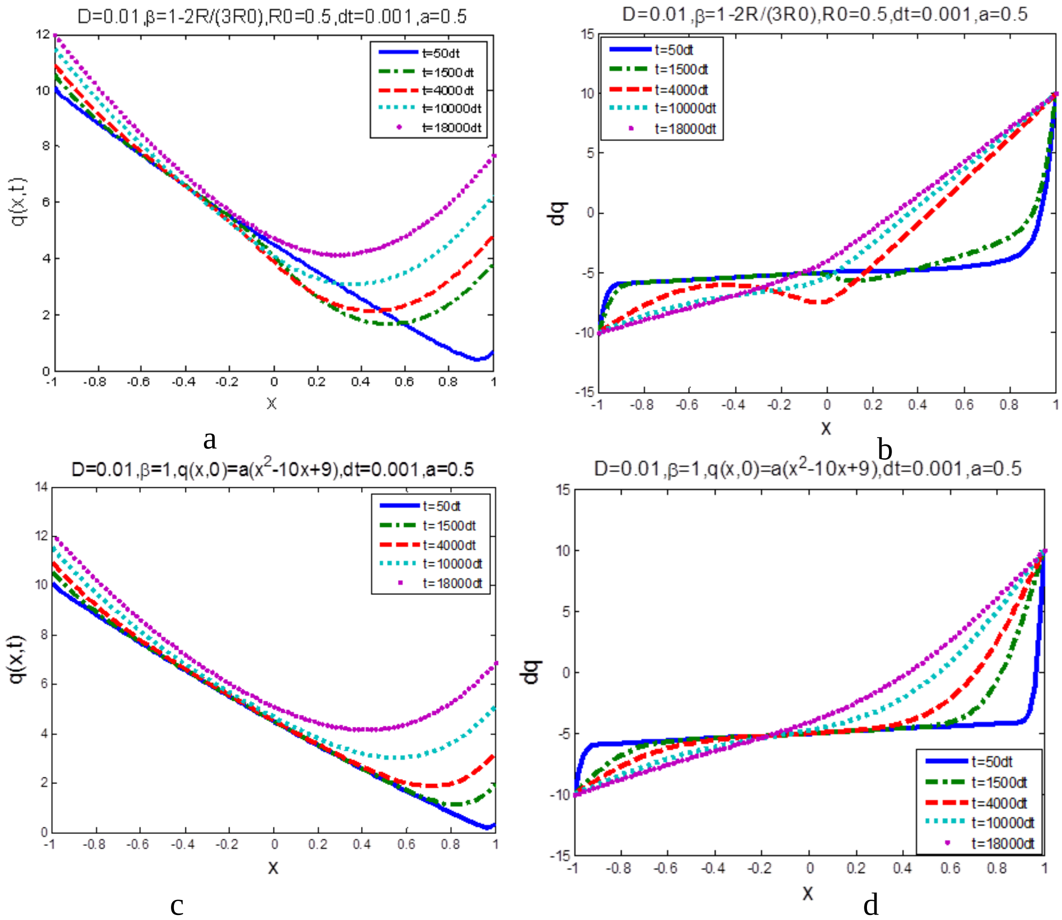
All this behavior taken together suggests that the concentration tends to accumulate on regions where the reactivity coefficient is high. The presence of the reactivity coefficient exerts a direct influence on the secondary flux and also an indirect influence on the primary. Note that these comments are consistent only for the case of diffusion of particles in a confined region.

Now let us examine what happens for different initial and boundary conditions. Let the initial condition be:

$$q(x,0)=a\left(x^2-10x+9\right),\qquad a=0.5$$

and the boundary condition:

$$\partial q(-1,t)/\partial x=-a*20=-10,\ \partial q(1,t)/\partial x=a*20=-10,\ \partial^3 q(-1,t)/\partial x^3=0,$$
$$\partial^3 q(1,t)/\partial x^3=0$$



a b c d

Fig.4.4Evolution of q and first derivative with flux into the domain for anisotripic medium comparing with classical model

With the prescribed boundary conditions the concentration in the domain will grow steadily since we have internal flux at both ends. The behavior for the two cases, the Fickian diffusion and the bi-flux diffusion will be very similar. However, some small but meaningful deviations are to be observed. While the densification process for the classical case follow a non decreasing path for all points in the interval [-1,1] Fig.4.4c. For the bi-flux process this is not true Fig.4.4a. In the interval [-0.2, 0.6] there is an initial reduction in the concentration. It is as if particles in this region were requested to concentrate at points close to $x=-1$. Note that the concentration at $x=-1$ grows quicker for the bi-flux process than for the classical one. This is certainly due to the perturbation on the primary flux and the presence of the secondary flux for the new approach, both introduced by the fourth order differential term. This phenomenon is similar to the case of the response to an initial condition concentrated on the origin as explained in the previous chapter. It confirms the hypothesis of the intense demand for particles when the bi-flux approach is taken to model the diffusion process. This happens for some particular conditions. For the present case it is compatible with the particle distribution.

Comparing Fig.4.4b with Fig.4.4d it is clearly seen that the specific primary flux intensity is higher for the bi-flux process than for the classical theory, particularly in the region [0,1]. The presence of the R(x) on that region also contributes to the acceleration of this kind of behavior.

Now there is not yet any observable phenomenon that has used this type of approach. Physico-chemical processes are difficult to devise that could follow the process proposed here. However it is not difficult to see that the motion of living organisms or certain species of animals are adequately modeled by the proposed theory. After the results obtained above it is reasonable to assume that the reactivity coefficient R may be associated to some kind of attractor representing food or some kind of pheromone. The introduction of this type of disturbance in the environment, substratum, will modify the natural diffusion process attracting the individuals toward regions where R is high. Therefore the model could satisfactorily represent the motion of certain types of organisms in the presence of some stimulus that could induce change in their energy states. In any case experimental confirmation is necessary to validate the process.

4.2 Diffusion processes on an active anisotropic substratum

The motivation induced from the solution above regarding the reactivity component as a possible attractor suggests taking into consideration an active role of that parameter. That is it is reasonable to consider the reactivity coefficient function of time, or more precisely, subjected to a given law that regulates its evolution in time. If we consider the reactivity factor as the food supply in a set of living organisms diffusing in some substratum the following system could be proposed to model the system:

$$\begin{aligned} \frac{\partial q(x,t)}{\partial t} &= \frac{\partial}{\partial x}\left(\beta D \frac{\partial q(x,t)}{\partial x}\right) - \frac{\partial}{\partial x}\left(\beta(1-\beta) R \frac{\partial^3 q(x,t)}{\partial x^3}\right) \\ \frac{\partial R(x,t)}{\partial t} &= D_R \frac{\partial^2 R(x,t)}{\partial x^2} \end{aligned} \tag{4.4}$$

That is we assume that the coefficient of reactivity evolves in time according to a diffusion process. If we think about food this means that the respective ingredients are able to spread in the medium. In the previous example the food would be restrict to a specific area.

Consider the system 4.4 Let D=0.1 and D_R=0.05. The initial distribution of the reactivity coefficient R(x,0) is the same as in the previous cases Fig.4.1. Let us consider for the following case the fraction β decaying exponentially with the reactivity coefficient R:

$$\beta = \exp\left(-5\left(\frac{R}{R_0}\right)^2\right) \quad \text{with} \quad R_0 = 5$$

The boundary conditions are:

$\partial R(-1,t)/\partial x = 0$ and $\partial R(1,t)/\partial x = 0$. For the main equation referring to the concentration q(x,t) the initial condition is defined as :

$q(x,0) = \exp\left(-10x^2\right)$ for all x such that $\exp(-10x^2) \geq 0.1$

$q(x,0) = 0.1$ for all x such that $\exp(-10x^2) < 0.1$

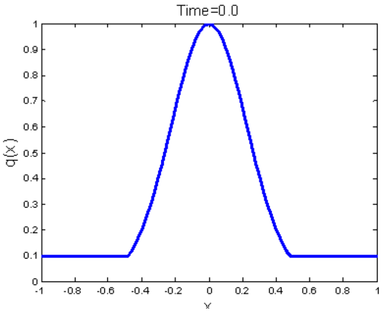


Fig 4.5 Initial distribution

Under this condition we approach an initial distribution concentrated around x=0 and avoid the possible negative values that could appear close to x=0, Fig.4.5

The boundary conditions correspond to a closed reservoir, no flux at the boundaries.

$$\left.\frac{\partial q}{\partial x}\right|_{x=\pm 1} = 0 \quad \text{and} \quad \left.\frac{\partial^3 q}{\partial x^3}\right|_{x=\pm 1} = 0$$

The numerical solution was performed with the cubic Hermit polynomials as base function for the BFS finite element method. The approximations for the reactive coefficient R is shown in table 6.a. Since the equation governing the evolution of R(x,t) is the classical second order partial differential equation the convergence is quite good. The results for N=40 elements and N=640 elements is less than 1%.

Table 4.1a Convergence for R(x,0.5)

N	R(-1, 0.5)	R(-0.5, 0.5)	R(0, 0.5)	R(0.5, 0.5)	R(1,0.5)
20	3.528e-006	0.00408447	0.54172842	2.89988673	1.07829432
40	3.592e-006	0.00408366	0.54172551	2.89991677	1.07807229
80	3.595e-006	0.00408364	0.54172550	2.89991695	1.07805816
160	3.595e-006	0.00408364	0.54172550	2.89991693	1.07805727
320	3.595e-006	0.00408364	0.54172550	2.89991693	1.07805722
640	3.595e-006	0.00408364	0.54172550	2.89991693	1.07805721

Tables 4.1b,c,d show the approximations for the concentration, the primary flux and the secondary flux in this order for time t=0.5. For points corresponding to the central part of the domain -0.5<x<0.5 the numerical solution converges rapidly for a limiting value for the three variables. Particularly for the concentration the convergence is very good

for all the domain of definition -1<x<1. For N=40 the stable value for q(x,0.5) is reached. For larger number of elements there is practically no gain. Only for primary and secondary fluxes the solutions are still subject to variations at x=1 and x=-1, but the values are so small that we may say that the convergence is quite satisfactory for all the range -1<x<1.

Table4.1b Convergence for q(x,0.5)

N	q(-1, 0.5)	q(-0.5, 0.5)	q(0, 0.5)	q(0.5, 0.5)	q(1,0.5)
20	0.12226478	0.27214696	0.39921318	0.37406883	0.36148479
40	0.12255830	0.27220083	0.39918163	0.37411394	0.36156123
80	0.12255088	0.27206392	0.39905445	0.37403083	0.36149358
160	0.12256879	0.27207399	0.39905950	0.37403900	0.36150301
320	0.12256860	0.27206662	0.39905266	0.37403457	0.36149943
640	0.12256956	0.27206680	0.39905257	0.37403478	0.36149975

Table4.1c Convergence for $\boldsymbol{\Psi}_1$ (x,0.5)

N	$\boldsymbol{\Psi}_1$ (-1, 0.5)	$\boldsymbol{\Psi}_1$ (-0.5, 0.5)	$\boldsymbol{\Psi}_1$ (0, 0.5)	$\boldsymbol{\Psi}_1$ (0.5, 0.5)	$\boldsymbol{\Psi}_1$ (1,0.5)
20	-1.263e-005	-0.05723163	0.00425233	0.00454377	-9.734e-007
40	-2.027e-006	-0.05713757	0.00425765	0.00453149	-1.568e-007
80	-2.691e-007	-0.05711297	0.00424832	0.00452536	-2.179e-009
160	-3.410e-008	-0.05710970	0.00424774	0.00452486	-2.819e-009
320	-4.278e-009	-0.05710838	0.00424713	0.00452454	-3.556e-010
640	-5.352e-010	-0.05710813	0.00424706	0.00452449	-4.456e-011

Table4.1d Convergence for $\boldsymbol{\Psi}_2$ (x,0.5)

N	$\boldsymbol{\Psi}_2$ (-1, 0.5)	$\boldsymbol{\Psi}_2$ (-0.5, 0.5)	$\boldsymbol{\Psi}_2$ (0, 0.5)	$\boldsymbol{\Psi}_2$ (0.5, 0.5)	$\boldsymbol{\Psi}_2$ (1,0.5)
20	-4.829e-008	-0.04370391	0.93803336	0.11154303	-8.021e-004
40	-6.265e-009	-0.04338993	0.94616815	0.11110317	-2.297e-004
80	-7.907e-010	-0.04337977	0.94647171	0.11105621	-3.829e-005
160	-9.900e-011	-0.04337640	0.94643840	0.11104825	-5.245e-006
320	-1.235e-011	-0.04337548	0.94642950	0.11104706	-6.724e-007
640	-1.644e-011	-0.04337524	0.94642610	0.11104665	-8.459e-008

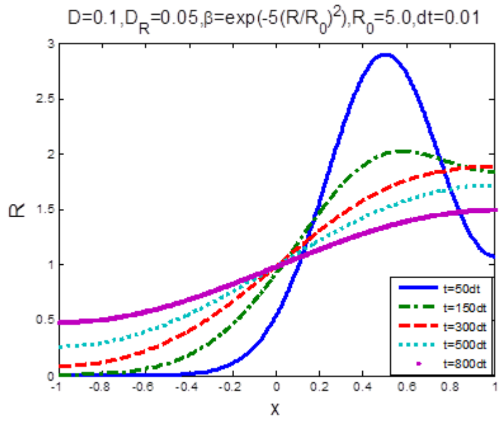


Fig.4.6a. Evolution of R

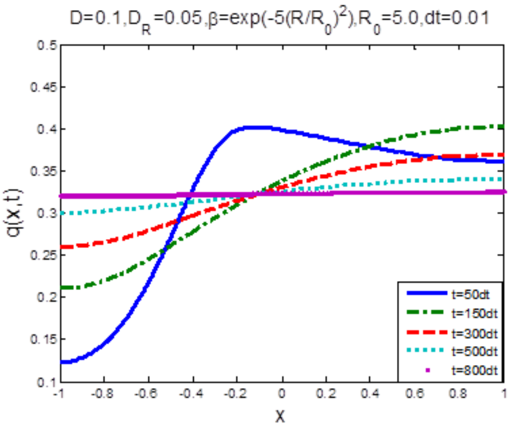


Fig.4.6b. Evolution of q

The evolution of R(x,t) and q(x,t) are given in Fig.4.6. It is interesting to observe that as expected the initially symmetric distribution is deviated towards the left. The concentration decreases quickly converging to the uniform distribution as expected from the theory. The nutrients accumulate on the right side since the flux is blocked at x=1. This behavior attracts the diffusing particles, supposedly living organisms, to the right end very quickly.

The diffusing fraction of particles in the primary energy state decays exponentially with R. But R also decreases as time increases since it is subjected to a diffusion process. There is partial compensation along this process. The solution converges to a steady state as can be also seen from Fig.4.7 representing the time variation of the concentration at three specific points:

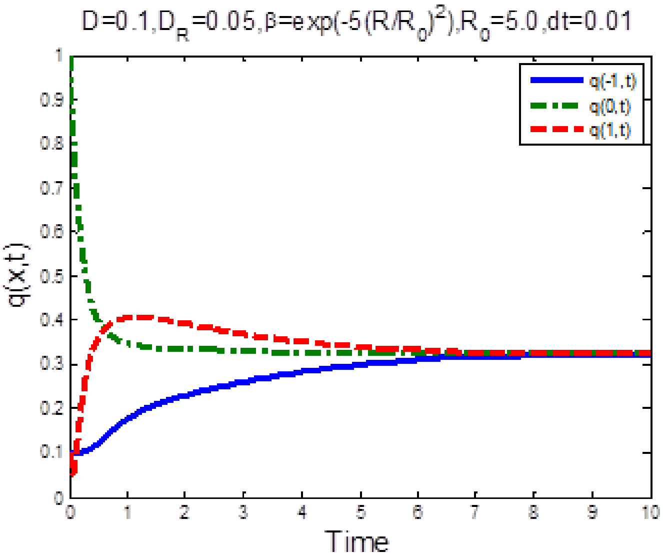


Fig.4.7 The evolution for *q(-1,t),q(0,t)* and *q(1,t)* for R without source term

The evolution of the concentration at x= 1 and x= −1 follow completely different paths. At x=1 close to the points where food accumulation increases rapidly the concentration grows more quickly than at x=−1. This is therefore a confirmation of the assumption that the reactivity coefficient for this case is compatible with the hypothesis of nutrients available for the living organisms. For sake of completeness Fig.4.8 shows the primary and secondary fluxes for the concentration. Now let us examine another interesting situation similar to the previous problem except that a “food” source is included in the

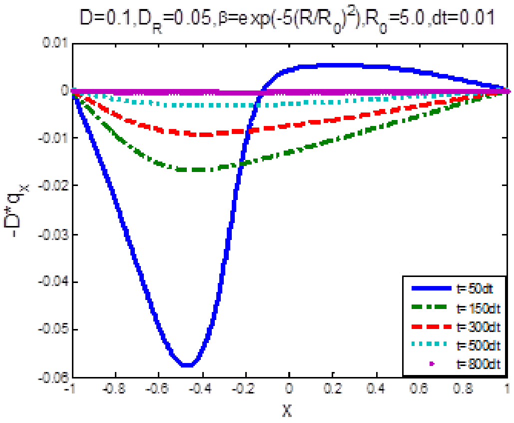


Fig.4.8a Evolution of first flux

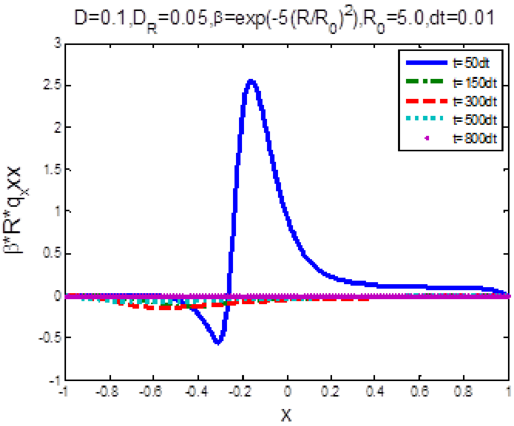


Fig.4.8b Evolution of second flux

formulation. That is the new system reads:

$$\frac{\partial q(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\beta D \frac{\partial q(x,t)}{\partial x}\right) - \frac{\partial}{\partial x}\left(\beta(1-\beta) R \frac{\partial^3 q(x,t)}{\partial x^3}\right)$$

$$\frac{\partial R(x,t)}{\partial t} = D_R \frac{\partial^2 R(x,t)}{\partial x^2} + A(R(x,t))$$

The term $A(R(x,t))$ represents a source of food. That is, there is limited source of nutrient proportional to the actual nutrient available. Take A=0.7 The solution was obtained with the same method described in the appendix as for the other cases.

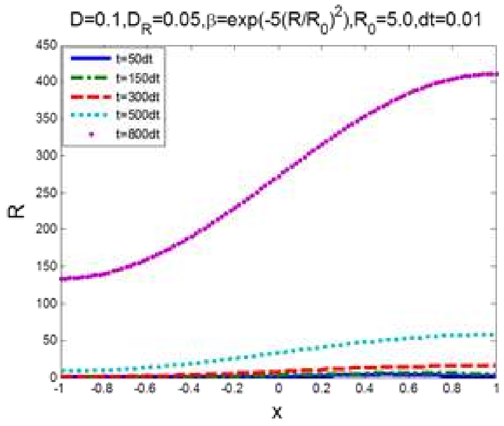


Fig. 4.9a Evolution of R

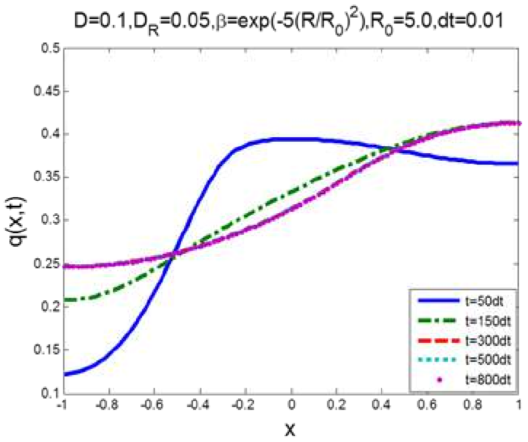


Fig. 4.9b Evolution of q

The solution for both variables q(x,t) and R(x,t) are displayed in Fig.4.9. The tendency for the concentration q(x,t) to deviate towards regions where R is large is again confirmed. The peculiarity of this solution refers to the limiting case where the solution tends to an abnormal steady state or freezes for a non uniform distribution. After a sufficient long time the concentration profile becomes a curve in the interval [−1.1]. The

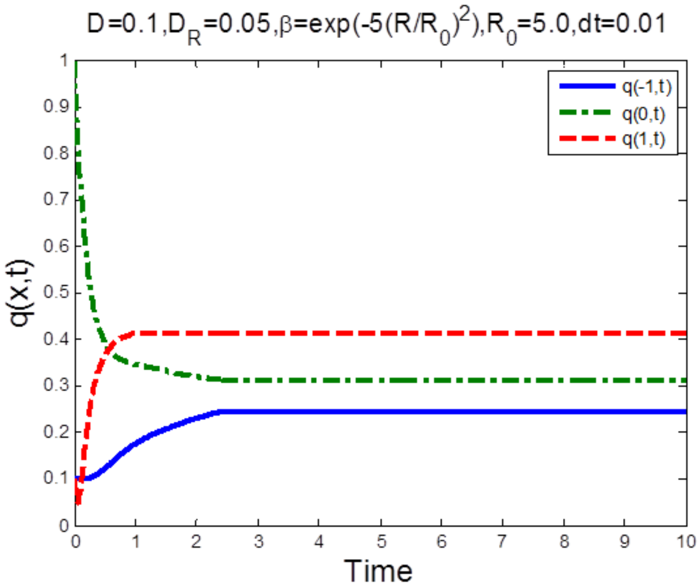


Fig.4.10 The evolution for *q(-1,t)*,*q(0,t)* and *q(1,t)* for R with source term

expected value for most of the cases for sealed domains, that is, no flux at the ends, will be a uniform distribution of the concentration $\lim_{t\to\infty} q(x,t) = const$. This however doesn't happen for this case. The concentration profile tends to curve as t→∞, as seen from Fig.4.9. According to the classical theory this is impossible. The reason that allows for this anomalous behavior is that the bi-flux theory depends critically from the fraction β of particles excited by the potential generating the primary flux. Note that the secondary flux doesn't exist if the primary flux is extinguished. But the fraction β is a decreasing function of R. When R→∞ then β→0 and there is no motion at all. The system becomes freeze in some peculiar energy state. Now in our problem we assumed a continuous source for the reactivity coefficient. Therefore R grows continuously and the fraction β approaches zero leading to a non uniform distribution of the concentration profile. The solution obtained is compatible with the theory and could not lead to a different result. Fig.4.10 shows the time variation of the concentration for three representative points , x=-1, x=0, x=1. The limiting values as t increases are different for the three points. At t≈3 the concentrations at these points reaches a limiting value and remain practically constant for all t > 3.

The convergence for t=0.5 referring to the approximations obtained for the reactivity coefficient, the concentration and the primary and secondary fluxes are displayed in the tables 4.2a,b,c,d. The same comments as for the previous case apply to this case.

Table4.2a Convergence for R(x,0.5) in the model for R with source term

N	R(-1, 0.5)	R(-0.5, 0.5)	R(0, 0.5)	R(0.5, 0.5)	R(1,0.5)
20	5.344e-006	0.00596787	0.77387164	4.11078831	1.54043215
40	5.439e-006	0.00596674	0.77386734	4.11083007	1.54011738
80	5.443e-006	0.00596671	0.77386732	4.11083031	1.54009735
160	5.443e-006	0.00596671	0.77386731	4.11083027	1.54009609
320	5.443e-006	0.00596671	0.77386731	4.11083027	1.54009601
640	5.443e-006	0.00596671	0.77386731	4.11083027	1.54009601

Table4.2b Convergence for q(x,0.5) in the model for R with source term

N	q(-1, 0.5)	q(-0.5, 0.5)	q(0, 0.5)	q(0.5, 0.5)	q(1,0.5)
20	0.12224443	0.27044148	0.39457073	0.37989942	0.36581108
40	0.12253791	0.27049543	0.39454170	0.37994117	0.36588350
80	0.12253048	0.27035807	0.39441406	0.37985815	0.36581709
160	0.12254839	0.27036817	0.39441928	0.37986608	0.36582642
320	0.12254821	0.27036078	0.39441242	0.37986166	0.36582291
640	0.12254916	0.27036095	0.39441234	0.37986184	0.36582323

Table4.2c Convergence for $\boldsymbol{\Psi}_1(x,0.5)$ in the model for R with source term

N	$\boldsymbol{\Psi}_1$ (-1, 0.5)	$\boldsymbol{\Psi}_1$ (-0.5, 0.5)	$\boldsymbol{\Psi}_1$ (0, 0.5)	$\boldsymbol{\Psi}_1$ (0.5, 0.5)	$\boldsymbol{\Psi}_1$ (1,0.5)
20	-1.217e-005	-0.05577710	-0.00031766	0.00482320	-6.561e-007
40	-1.980e-006	-0.05568149	-0.00031754	0.00480914	-8.917e-008
80	-2.635e-007	-0.05565664	-0.00032750	0.00480242	-1.190e-008
160	-3.342e-008	-0.05565342	-0.00032793	0.00480189	-1.523e-009
320	-4.193e-009	-0.05565209	-0.00032853	0.00480153	-1.915e-010
640	-5.245e-010	-0.05565184	-0.00032858	0.00480148	-2.398e-011

Table4.2d Convergence for $\boldsymbol{\Psi}_2(x,0.5)$ in the model for R with source term

N	$\boldsymbol{\Psi}_2$ (-1, 0.5)	$\boldsymbol{\Psi}_2$ (-0.5, 0.5)	$\boldsymbol{\Psi}_2$ (0, 0.5)	$\boldsymbol{\Psi}_2$ (0.5, 0.5)	$\boldsymbol{\Psi}_2$ (1,0.5)
20	-5.939e-008	-0.06563441	0.57574594	0.10320541	-1.769e-004
40	-9.681e-009	-0.06769771	0.57579652	0.10221345	-8.951e-005
80	-1.221e-009	-0.06768774	0.57543121	0.10210151	-1.574e-005
160	-1.528e-010	-0.06768246	0.57537589	0.10208880	-2.180e-006
320	-1.908e-011	-0.06768105	0.57536587	0.10208719	-2.802e-007
640	-3.234e-012	-0.06768068	0.57536342	0.10208677	-3.528e-008

Chapter 5

Bi-Flux Diffusion on 2D Anisotropic Domains

Let us turn now to the diffusion problem in a two dimensional space domain $\mathbf{R}^2$. The diffusion problem for the bi-flux diffusion state is rather complex not only because it requires the definition of two new coefficients, the fraction β and the reactivity coefficient R, or one of them plus a functional relationship between these two parameters, but also as seen in the previous chapter the proper choice of the secondary flux potential. Since this a new approach and the theoretical/numerical development up to now has open several research windows we decided to explore the possible new behaviors induced by some possible choices of the new coefficients. Note that all the problems posed in the next sections are linear problems. Even for those cases there are considerable large possibilities of peculiar behaviors. As a matter of fact a more precise mathematical modeling even leading to linear equations is sometimes more effective than introducing non-linearity.

5.1. Asymmetric Anisotropy

Consider now the diffusion process taking place in a two dimensional domain defined by $[-1,1]\times[-1,1]$. Let us initially assume the secondary flux given by $\mathbf{\Psi}_2^{(3)}$ then the corresponding differential equation reads:

$$\frac{\partial q}{\partial t} = \nabla\cdot(\beta D\nabla q) - \nabla\cdot((1-\beta))R\nabla(\nabla\cdot(\beta\nabla q))$$

The medium is anisotropic in the sense that the reactivity varies as a function of x.

$R(x,y) = R_0 x + 0.001 \qquad 0 \le x \le 1,\ -1 \le y \le 1 \qquad R_0 = 5$

$R(x,y) = 0.001 \qquad -1 \le x < 0,\ -1 \le y \le 1$

Fig.5.1b shows the picture of R in the domain. The diffusion coefficient is constant D=0.1. The initial condition, as shown in the Fig.5.1a, is given by:

$$q(x,y,0) = \exp\left(-10x^2 - 10y^2\right)$$

And the boundary conditions impose no flux, primary and secondary, at the boundaries:

$$\nabla q\big|_{y=\pm 1} = 0 \qquad \nabla q\big|_{x=\pm 1} = 0 \qquad \nabla \Delta q\big|_{y=\pm 1} = 0 \qquad \nabla \Delta q\big|_{x=\pm 1} = 0$$

The correlation between β and R will be assumed to be linear as given by:

$\beta = 1 - \gamma R / R_{\max}$ with $R_{\max} = 5.001$

The function $\beta = \beta(x,y)$ is displayed in Fig.5.1c.

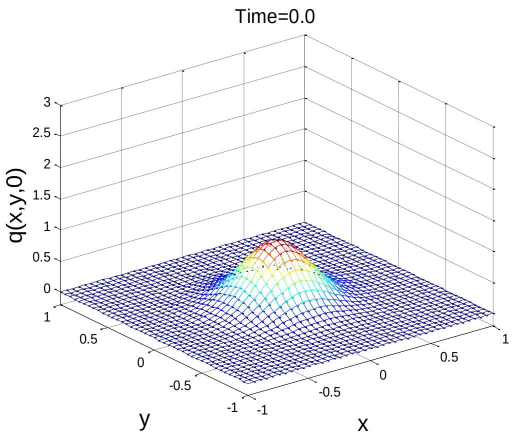


Fig.5.1a Initial distribution

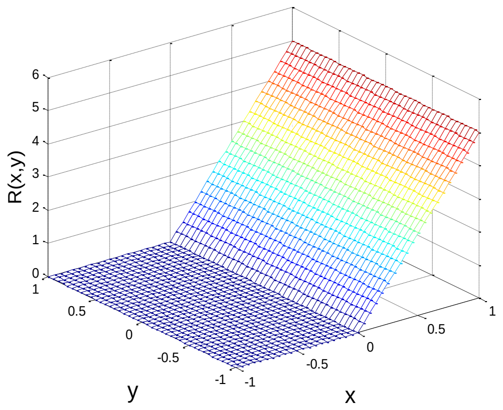


Fig.5.1b Reactivity coefficient

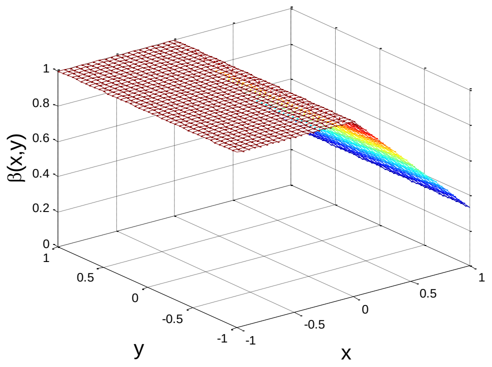


Fig.5.1c The fraction β

The solution was obtained numerically with the Bogner-Fox-Schmidt (BFS) (Bogner, 1965) finite element method on a mesh composed of square elements and the Hermite polynomials as base functions (Irons, 1969; Petera, 1994; Watkins, 1976). The time integration was performed with a Euler backwards difference procedure. The convergence was satisfactory as shown in table 5.1.

Table 5.1. Convergence of concentration for five points in 2D, with linear relationship

N*N	q(-1,-1, 0.01)	q(-0.4,0,0.01)	q(0, 0,0.01)	q(0.4, 0,0.01)	q(1.0,1.0,0.01)
10*10	-2.6275e-006	0.2088183	0.8099417	0.2741395	-0.0882347
20*20	1.0999e-008	0.2064627	0.8328648	0.2706597	-0.0877910
40*40	1.1182e-008	0.2064486	0.8533093	0.2686040	-0.0872301
80*80	1.1199e-008	0.2064486	0.8649527	0.2679241	-0.0869223

The solution confirmed the tendencies found in the previous cases for one-dimensional diffusion. The concentration tends to increase more rapidly in the regions where the reactivity coefficient is high. The initial symmetry is clearly broken as can be seen from Fig.5.2. The concentration distribution grows asymmetrically with respect to the x direction.

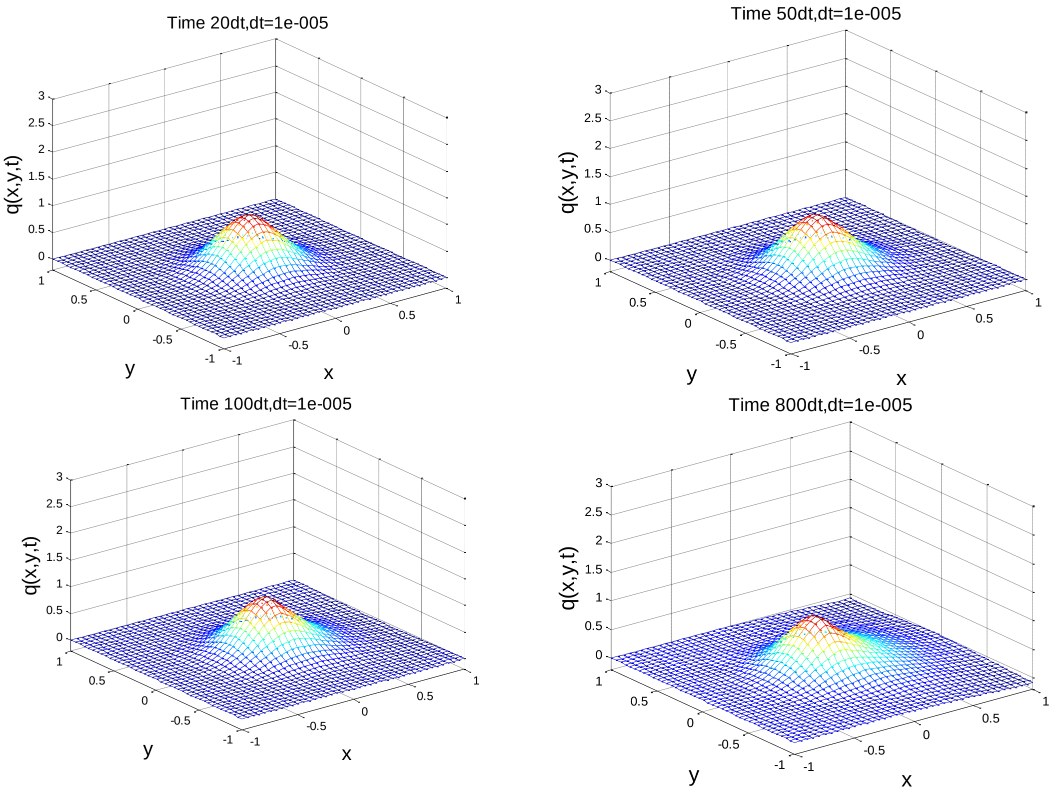


Fig.5.2 Evolution of concentration

Fig.5.2 shows the contour lines of the concentration in the domain $[-1,1]\times[-1,1]$ corresponding to the surfaces displayed in Fig.5. We can see that the higher level contour lines deviate to the right which indicates that particles are moving preferably to the right side. That is, the region where the reactive factor increases exerts a kind of attraction effect on the particle path.

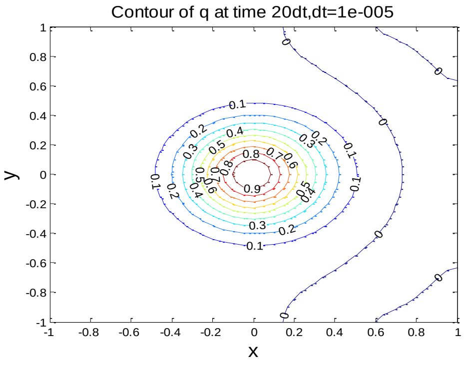


Fig.5.3a Contour of q at time 20dt

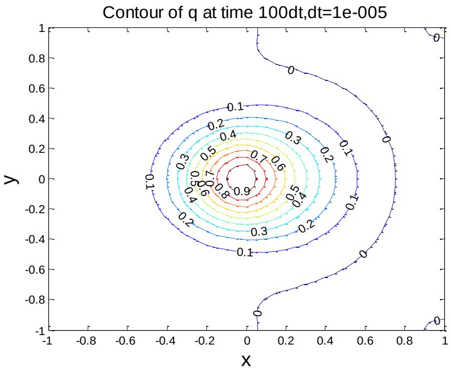


Fig.5.3b Contour of q at time 100dt

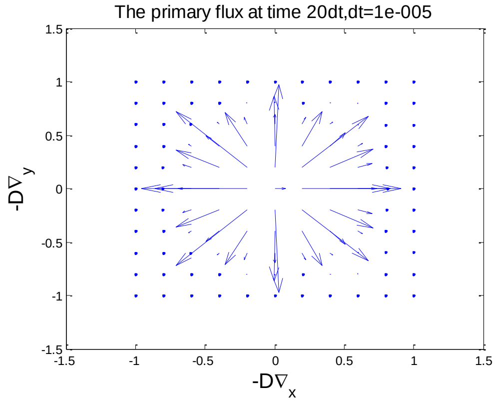


Fig.5.4a The primary flux at 20dt

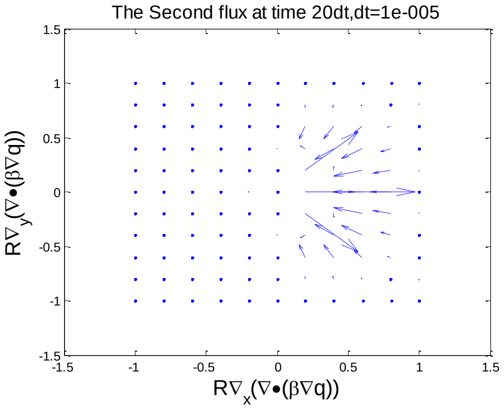


Fig.5.4b The second flux at 20dt

The figures 5.4a, b and 5.5a, b show the primary and secondary fluxes at two different times 20dt and 800dt, respectively. At very short times, Fig.5.4b, the secondary flux becomes very high close to the central point [0,0] where the density is maximum pushing particles toward the border. For points far from the center [0,0] there is an inversion of the secondary flux direction pulling particles towards the center. This behavior seems to be typical when the initial condition is highly concentrated around a point, a kind of pulse. For the case of one dimension problems this behavior was already

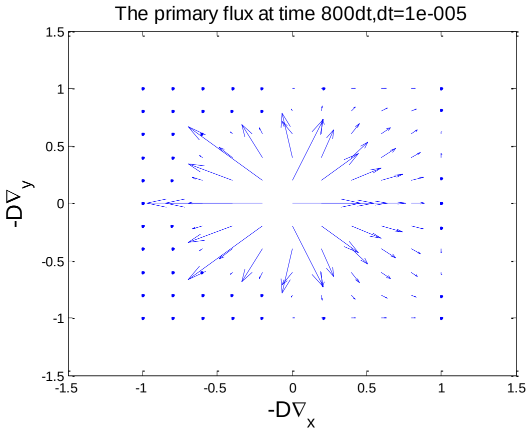


Fig.5.5a The primary flux at 800dt

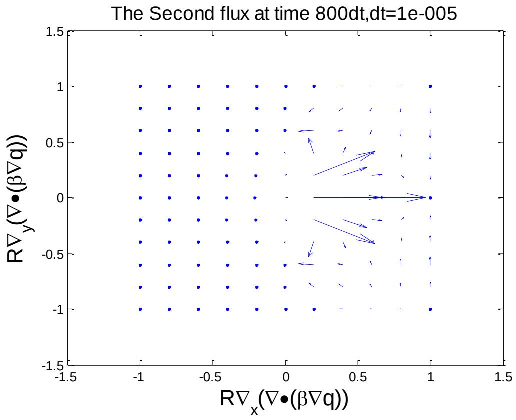
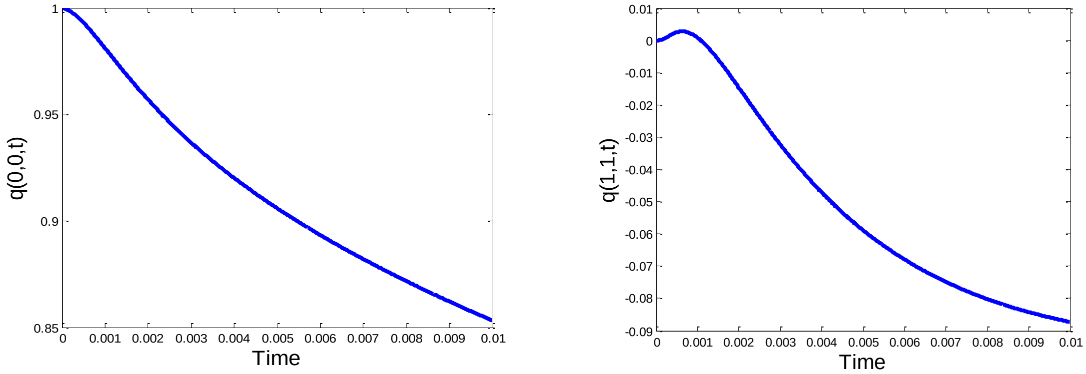


Fig.5.5b The second flux at 800dt

discussed in chapter 3. The peculiarity for the present solution is that there is no symmetry due to the variation of the reactivity factor with x,y. The inversion of flux direction appears for the region x>0. After a sufficiently long time t=800dt the flux is stabilized in just one direction pushing particles to the right border. Note that the secondary flux is inexpressive for x<0.

The primary flux presents a more regular behavior. Initially t=20dt it is practically symmetric with respect to the x axis. As time increases, however, an asymmetric pattern starts to appear showing the influence of the bi-flux behavior also on the primary flux distribution.

Another typical behavior of the bi-flux approach that is governed by a fourth order partial differential equation is the growth of negative values of the concentration at some critical points. For the present problem the negative value of the concentration grows at the corners [1,1] and [1,-1] as indicated in the Fig.5.3b and 5.6-b. After an initially accumulation of particles at the referred points the evolution of the concentration shows a rapidly decrease of the concentration towards negative values. The relatively intense particle flux imposed by the secondary flux pulling particles towards the center request particle from the corners [1,1] and [1,-1] generating this phenomenon. The concentration at the central point [0,0] decreases steadily as expected Fig.5.6a.



(a) (b)

Fig.5.6 Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t)* for $\boldsymbol{\Psi}_2^{(3)}$ with $\gamma = 2/3$

Now it is also important to test the solution for a different definition of the secondary flux. For the previous solution the secondary flux was defined as the third class:

$$\boldsymbol{\Psi}_2^{(3)} = R\Delta\left(\beta\nabla q\left(x,y,t\right)\right)$$

Now let us see what happens if we take the second flux defined as:

$$\boldsymbol{\Psi}_2^{(2)} = R\nabla\left(\beta\Delta q\left(x,y,t\right)\right)$$

This definition, as explained before, is probably more consistent with what is to be expected for the definition of flux potential. It correlates the potential with the gradient of the curvature of the density distribution. With this definition the governing equation reads:

$$\frac{\partial q}{\partial t} = \nabla\cdot\left(\beta D\nabla q\right) - \nabla\cdot\left(\left(1-\beta\right)\right)R\nabla\left(\beta\Delta q\right)$$

For this case the perturbation introduced in the primary flux by the secondary flux is not so critical as for the third class definition. The intital and boundary considitons are the same as for the previous problem and the reactive coefficient *R* and its correlation with the fraction β, as well.

The solution for this case didn't present any important deviatios from the preceding case. Fig. 5.7a,b show the time variation of two representatives point, namely [0,0] and [1,1] for the previous case $\boldsymbol{\Psi}_2^{(3)}$ for diferent values of γ in the expression $\beta = 1 - \gamma R/R_{\max}$ with $R_{\max}$ = 5.001. Clearly the process is accelerated for increasing values of γ.

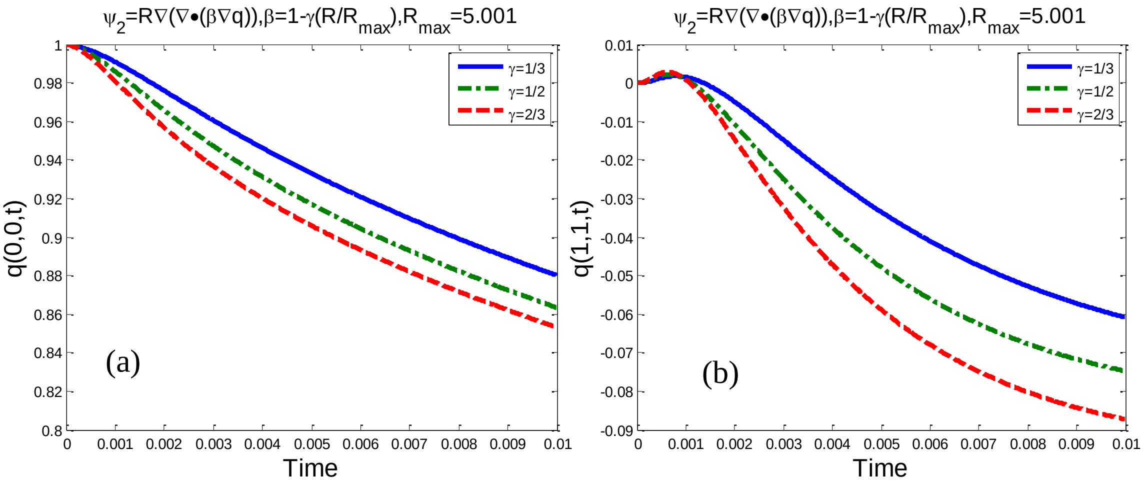


Fig.5.7 Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t)* for $\boldsymbol{\Psi}_2^{(3)}$

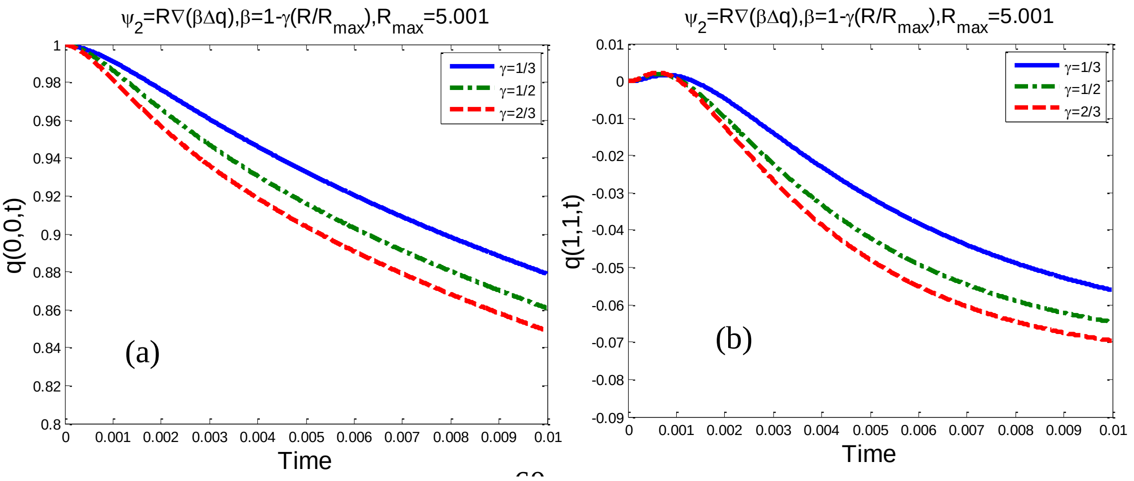


Fig.5.8 Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t)* for $\boldsymbol{\Psi}_2^{(2)}$

The solution for the secondary flux defined with the secondary class option doesn't differ essentially from the previous case except that the speed of variation of the density at the corners is considerably smaller for the second class flux as can be seen by comparing the figures 5.7b and 5.8b.

5.2. Axisymmetric anisotropy

For the second problem let us consider a new relationship between the reactivity *R* coefficient and the diffusing fraction of particles β excited in the primary energy state. Let

$$\beta = \exp\left(-\alpha\left(R/R_0\right)^2\right)$$

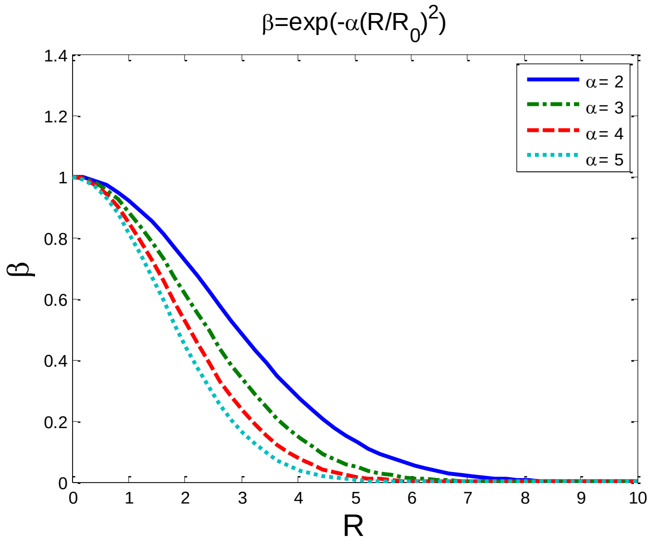


Fig.5.9 the exponent relationship between β and R

The exponential law is more flexible allowing for a large range of variation for R with a practical cutting effect for large values of time.

The problem is defined in a 2-D space within the region [1,-1]x[-1.1]. Let us take for the secondary flux the third class definition $\mathbf{\Psi}_2^{(3)} = R\Delta\left(\beta\nabla q(x,y,t)\right)$ leading to the equation:

$$\frac{\partial q}{\partial t} = \nabla\cdot\left(\beta D\nabla q\right) - \nabla\cdot\left(\left(1-\beta\right)R\Delta\left(\beta\nabla q\right)\right)$$

The initial condition admits a polar symmetric distribution, the same as in the problem 3.1 :

$$q(x,y,0)=\exp\left(-10x^2-10y^2\right)$$

together with the same boundary conditions. No flux, primary and secondary, at the boundaries:

$$\nabla q\big|_{y=\pm1}=0 \qquad \nabla q\big|_{x=\pm1}=0 \qquad \nabla\Delta q\big|_{y=\pm1}=0 \qquad \nabla\Delta q\big|_{x=\pm1}=0$$

The correlation between β and R will be assumed to be exponential given by:

$$\beta(R)=\exp\left(-\alpha(R/R_0)^2\right)$$

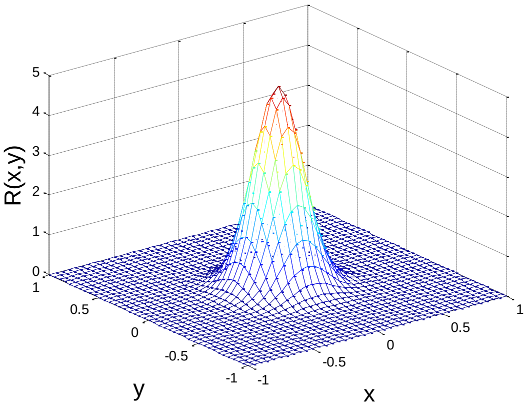


Fig.5.10a Reactivity coefficient

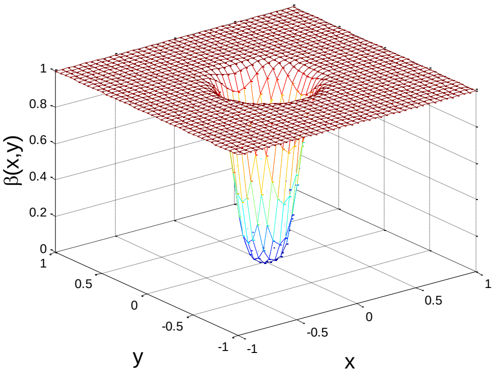


Fig.5.10b The fraction β

The reactivity coefficient is the same as in problem 5.1: $R(x,y)=5\exp\left(-10x^2-10y^2\right)$ and the fraction β is given by: $\beta(R)=\exp\left(-5(R/R_0)^2\right)$ with R_0=5, $\alpha=5$. Fig.s 5.10a and 5.10b show the functions R=R(x,y) and β=β(x,y). The diffusion coefficient is D=0.1.

The solution was obtained numerically as mentioned for the problem in chapter 3. The convergence as shown in the table 5.2 at time 0.01 is satisfactory.

Table 5.2Convergence of concentration for five points in 2D, with exponent relationship

N*N	q(-1,-1, 0.01)	q(-0.4,0,0.01)	q(0, 0,0.01)	q(0.4, 0,0.01)	q(1.0,1.0,0.01)
10*10	5.1377e-007	0.2365930	1.4844618	0.2365930	5.1377e-007
20*20	1.0887e-008	0.2266660	2.2950605	0.2266660	1.0887e-008
40*40	1.1193e-008	0.2265916	2.3408640	0.2265916	1.1193e-008
80*80	1.1210e-008	0.2265744	2.3375152	0.2265744	1.1210e-008

The evolution of the concentration is shown in Fig.5.11. Now this type of “diffusion” is peculiar and may represent one of the most important anomalies introduced by the bi-flux approach. Deviating from any expected evolution previewed by the classical theory the concentration q(0,0,t) is increasement instead of decreasement. Particles flow opposing the concentration gradient in the very beginning. It is kind of initial shock.

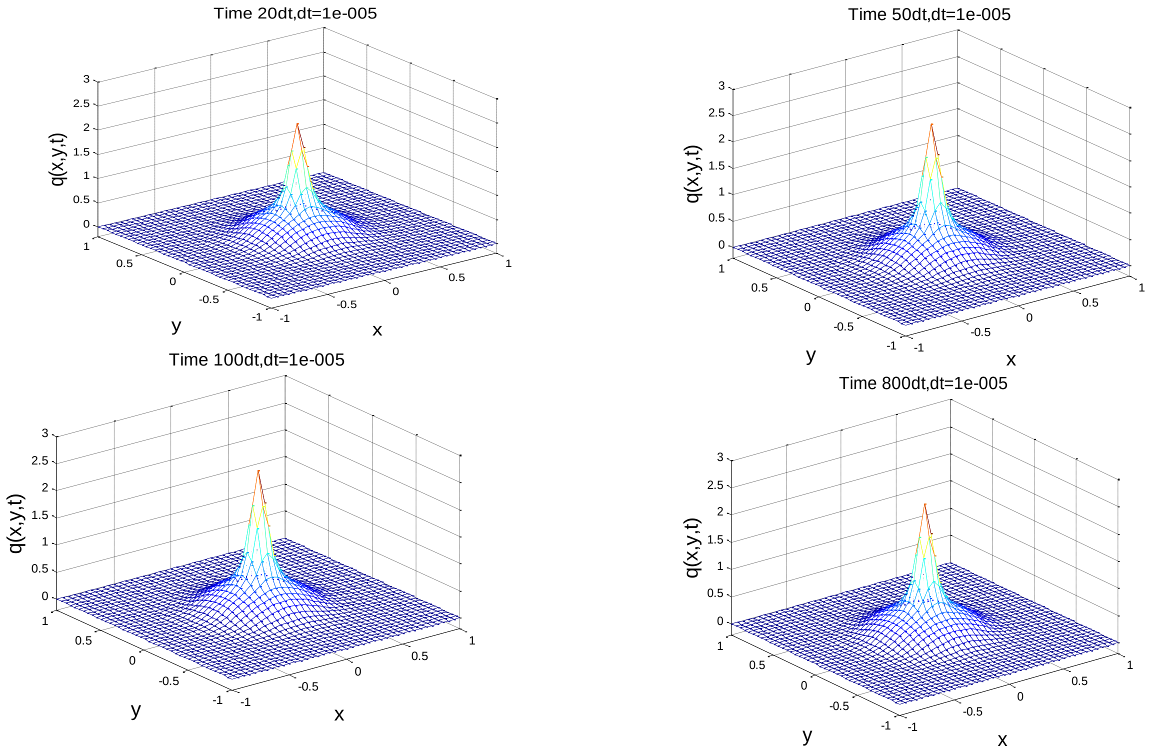


Fig. 5.11 Evolution of the concentration profile

Fig.5.12 represents the contour lines relative to the concentration distribution on the field of definition of the problem. As expected, the symmetry is preserved and no anomaly associated to negative values of q(x,y,t) is present for this problem. As this type of anomaly grows up immediately after the initial condition is imposed to the system, it is expected that the concentration will remain positive for all time is all over the domain.

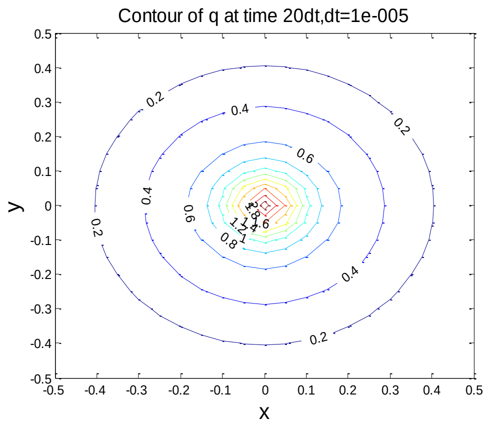


Fig.5.12a Contour of q at time 20dt

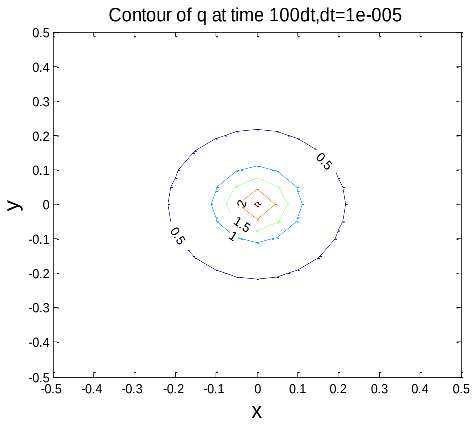


Fig.5.12b Contour of q at time 100dt

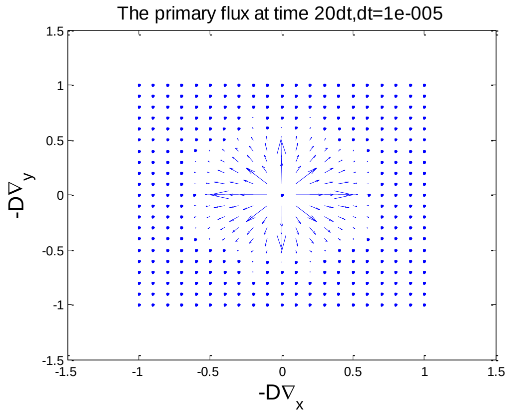


Fig.5.13a. The primary flux at 20dt

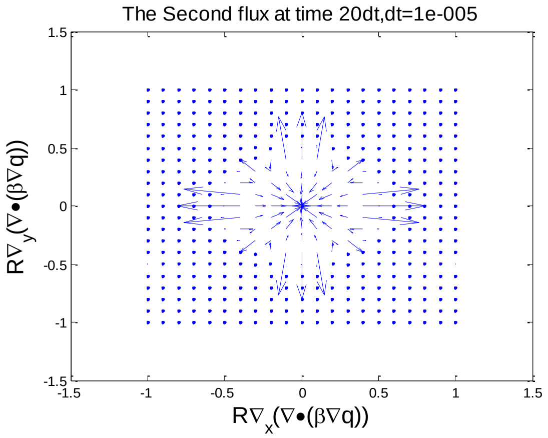


Fig.5.13b The second flux at 20dt

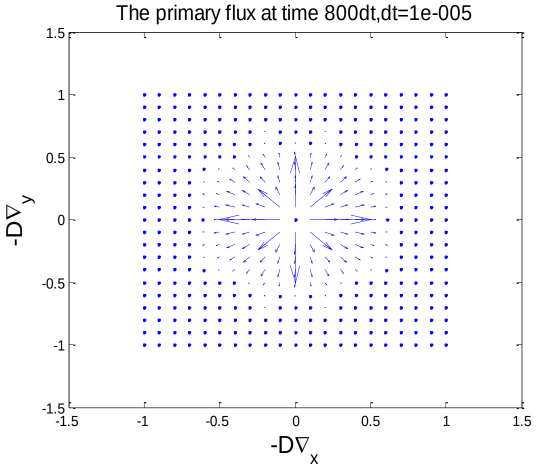


Fig. 14a The primary flux at 800dt

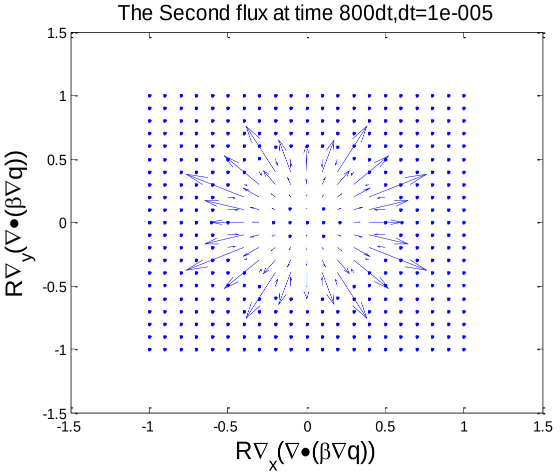


Fig.14b The second flux at 800dt

The primary and the secondary flux distributions for t=20dt and 800dt are shown in figures 5.13 and 5.14. The primary flux is regular with no peculiar disturbance from the expected behavior. It follows regularly the scattering process as expected from the Fick's law. The intensity of course depends on the physics imposed by the bi-flux diffusion process.

The secondary flux however presents a peculiar behavior consistent with the density variation in time. Note that immediately after the initiation of the process, that is, for short times, t< t* the secondary flux close to the center [0,0], that is inside a disk r< r* is negative pushing the particles towards the center. Outside this disk, that is for r>r* the secondary flux is positive contributing to the dispersion of particles as imposed also by the primary flux. This behavior is opposed to the flux distribution in space for the isotropic diffusion process. Indeed, after imposing a highly concentrated distribution, centered at the origin x=0, for t=0, the initial condition, the secondary flux excited close to the origin, x<x*, is positive and negative for x>x*. This behavior was considered as partly responsible for the negative values of the concentration on a limited region along the x axis. For the present case the situation is reversed and no negative values of the concentration appears in the solution. Therefore all the results obtained confirm the hypothesis that the negative values of the concentration are imposed by the secondary flux fluctuation around the central point of a kind of pulse as the initial condition.

Note also that after a sufficient long time the secondary flux vanishes inside a disk r<r**. the primary flux however remains active.

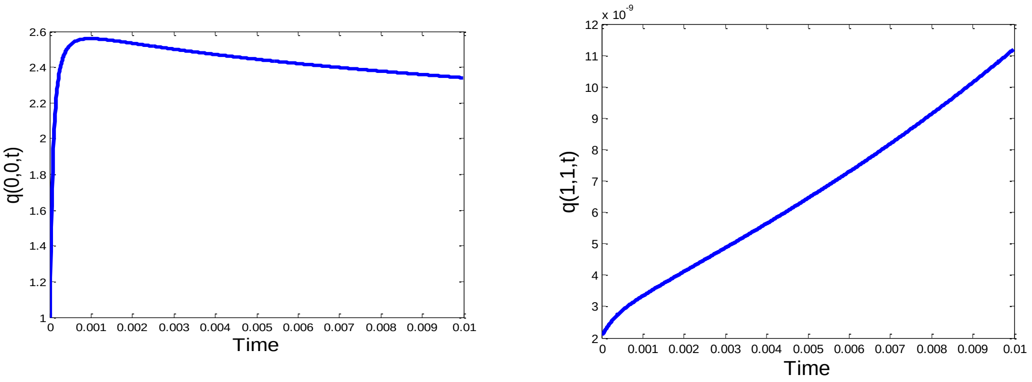


Fig. 5.15 Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t)* for $\boldsymbol{\Psi}_2^{(3)}$ with $\alpha = 5$

The Fig. 5.15 shows the rapid increase of the concentration at [0,0] starting from q(0,0,0)=1 to q(0,0,0.001) ≈ 2.6 representing a increase of 260%. Note also that for the corner [1,1] the concentration increases steadily. No negative value is expected.

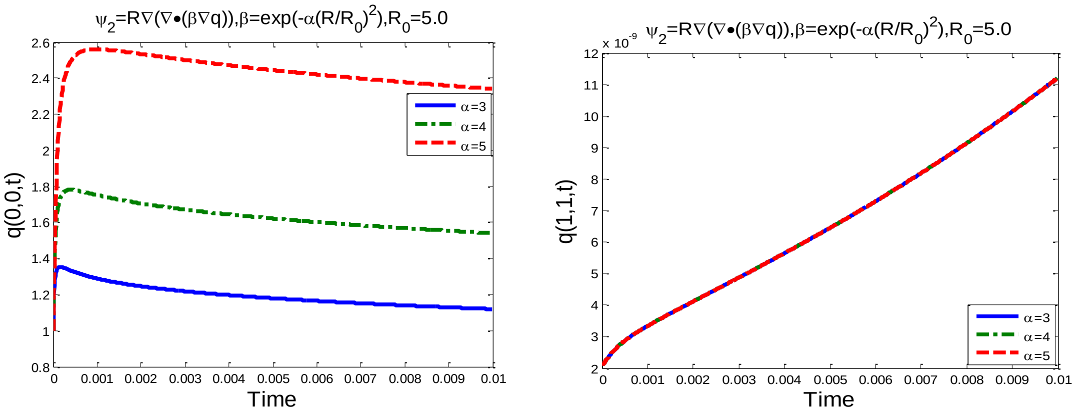


Fig 5.16. Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t)* for $\boldsymbol{\Psi}_2^{(3)}$ with $\alpha = 3,4,5$

The influence of the constant α in the exponential function relating R and β is shown in Fig. 5.19. The value of α affects the maximum value of the concentration and the respective time taken to reach the maximum as well. If α decreases from 5 to 3 the maximum of the concentration in the “diffusion” process will drop from 2.58 to 1.35. The maximum is very sensitive to the value of α. For other points the constant α practically doesn’t exert any substantial influence as sown in the figure 5.16b for the corner [1,1].

It is worthwhile comparing the solutions for a different option for the secondary flux potential. Let us take the secondary flux potential defined by:

$$\mathbf{\Psi}_2^{(2)} = R\nabla(\beta\Delta q(x,y,t))$$

The corresponding differential equation reads:

$$\frac{\partial q}{\partial t} = \nabla(\beta D\nabla q) - \nabla((1-\beta))R\nabla(\beta\Delta q)$$

Keeping all the other conditions as previously the solution referring to the central point q(0,0,t) and to the corner q(1,1,t) are displayed in the figure 5.17

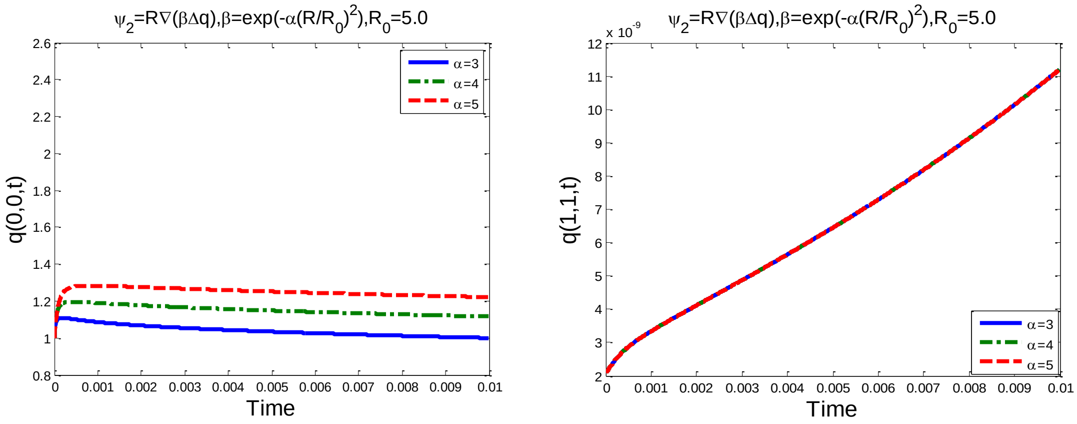


Fig 5.17 Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t)* for $\mathbf{\Psi}_2^{(2)}$ with $\alpha = 5,4,3$

The influence of the definition of the secondary flux potential is extremely important. The general trend of the concentration evolution is preserved, however the intensity is drastically reduced. For the constant α=5 the maximum at [0,0] reaches the value of 1.3 almost twice less than the value corresponding to the third class potential flux. This is a considerable difference. The reason, as explained before, is to be attributed to the perturbation on the primary flux imposed by the secondary flux. The influence of the second class flux potential is less critical than the influence attributed to the third class potential. The concentration in the corners varies according to the common trajectory characteristic of the others solutions.

In any case the problems posed above provide an unambiguous indication that the reactivity coefficient may work like an attractor, forcing the flux to converge to points where R(x,y) is maximum. The question now arises if there is any possible real situation that matches the behavior obtained with the theoretical results.

The motion of living organisms on a substratum where the reactivity factor plays the role of given nourishment may be a good example that fits the behavior previewed by the solution above. If the food is concentrated in a small region, with R(x,y) high, the organisms (particles) will displace towards that region where the probability to find food is high. This behavior is satisfactorily modeled by the above equations at least form the qualitative point of view. As already remarked the bi-flux approach is very much adequate to model the motion of cells or other entities that are able to change energy states. Living organisms usually carry this ability.

It is also puzzling that the Bose-Einstein condensate presents the same aggregation particularity where the velocity distribution of elementary particles tends to evolve according to similar distribution as shown in the figure 5.11.

Finally let us see how the solution is affected if the reactivity coefficient is a function of time. Consider the problem defined with the third class of secondary flux, that is, the potential that introduces the strongest perturbation on the concentration distribution. Take $R = R_0 \exp\left(-20x^2 - 20y^2 - 10t\right)$ with R_0=5.

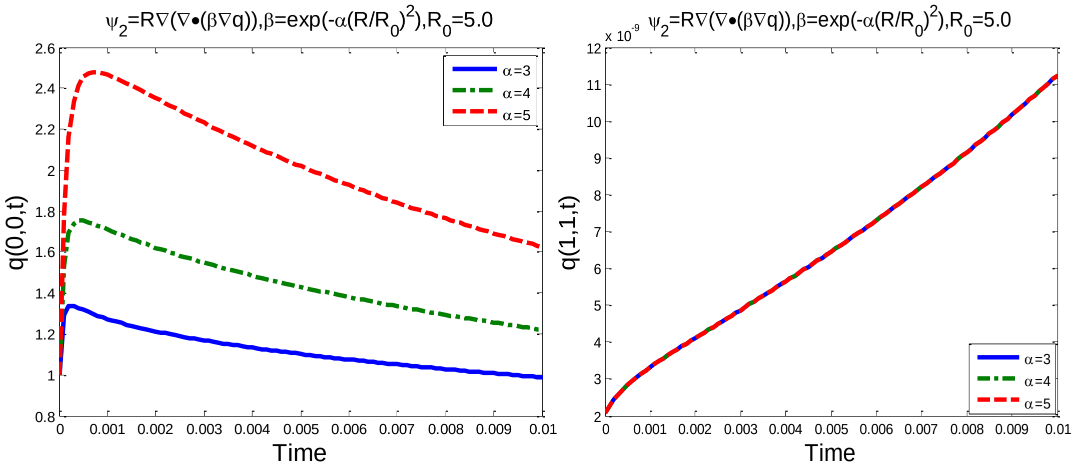


Fig 5.18. Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending domain and time, for $\mathbf{\Psi}_2^{(3)}$ with $\alpha = 5,4,3$

The Fig.5.18 shows clearly the influence of R as a decreasing function of time. As expected the decaying process is accelerated since R decreases in time. It is also clear that the maximum values reached by the concentration are smaller than the corresponding ones for a time independent reactivity coefficient. The time to reach the maximum density is also larger for R as decreasing function of time. Again we see another strong indication that the reactivity coefficient works as an attractor. If R decreases its capacity to attract the particles is reduced and the concentration tends also to decrease at an equivalent speed. The strong influence is at the middle. Other regions far from the center will be less affected proportionally to their distance from the origin. The evolution of the density at the corners will not be affected by the new function R(x,y,t).

For the case corresponding to the second class flux potential the time variation proposed for the reactivity coefficient doesn't introduce any substantial modification as shown in the Fig.5.19.

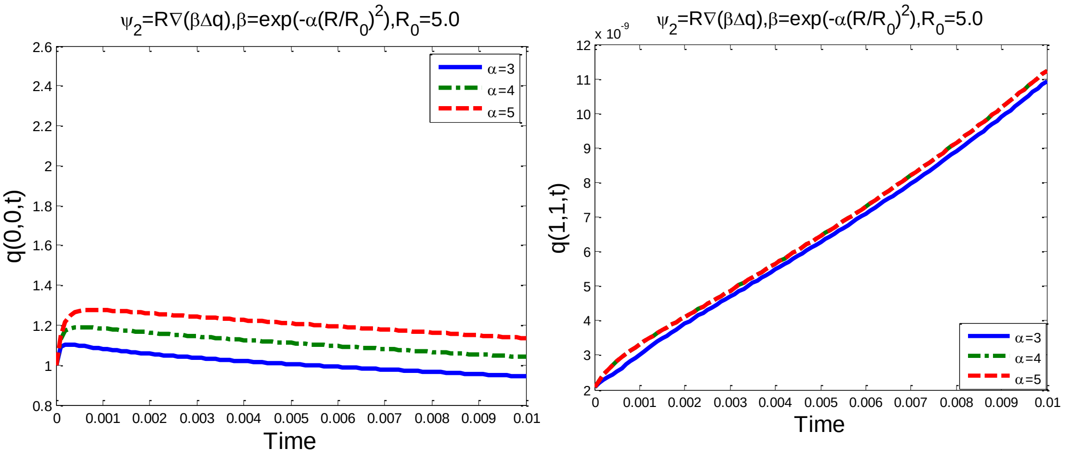


Fig. 5.19 Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending domain and time, for $\mathbf{\Psi}_2^{(2)}$ with $\alpha = 5,4,3$

5.3. Axisymmetric active anisotropy

One of the possible applications of the theory presented here, as already said, and is the motion of living organisms. Assuming this hypothesis and from the indications obtained from the behavior of the solution to the previous problems, it is admissible to associate the reactivity coefficient with food. But for several cases, particularly referring to micro-organism, the nourishment is a compound that is able to diffuse in the same substratum. Thus it is reasonable to admit Fick´s law governing the evolution of R:

$$\frac{\partial R(x,y,t)}{\partial t} = D_R \Delta R(x,y,t) \qquad (5.1)$$

It is therefore convenient to study the coupled system consisting of two diffusion process involving q(x,y,t) and R(x,y,t). The problem is defined in the same domain $[-1,1]\times[-1,1]$ as in the previous section and the boundary and initial conditions as well. Also the primary fraction β is an exponential function of R as before:

$$\beta = \exp\left(-\alpha (R/R_0)^2\right) \qquad \text{with } R_0=5$$

Now let us assume to solve (5.1) the following auxiliary data:

Boundary conditions: $\nabla R\big|_{boundary} = 0$

Initial condition: $R(x,y,0) = 5\exp\left(-10x^2 - 10y^2\right)$

The problem will be solved for various values of D_R: D_R=0.01, D_R=0.05 and D_R=0.1 to estimate the influence of this coefficient in the solution.

The diffusion coefficient D =0.1 is constant for all cases. Then let us consider the system:

$$\begin{aligned}&\frac{\partial q(x,y,t)}{\partial t} = \nabla\cdot(\beta D\nabla q(x,y,t)) - \nabla\cdot(R\beta(1-\beta)\nabla(\Delta q(x,y,t)))\\&\frac{\partial R(x,y,t)}{\partial t} = D_R\Delta R(x,y,t)\end{aligned} \tag{5.2}$$

The secondary flux is assumed to be generated by the first class potential:

$$\boldsymbol{\Psi}_2^1 = R(x,y,t)\beta\nabla(\Delta q(x,y,t))$$

The initial and boundary conditions are the same as in the previous section.

Fig.5.20a, 5.20b and 5.20c show the evolution of q(x,y,t) for two characteristic points, the central point q(0,0,t) and the corner q(1,1.t).

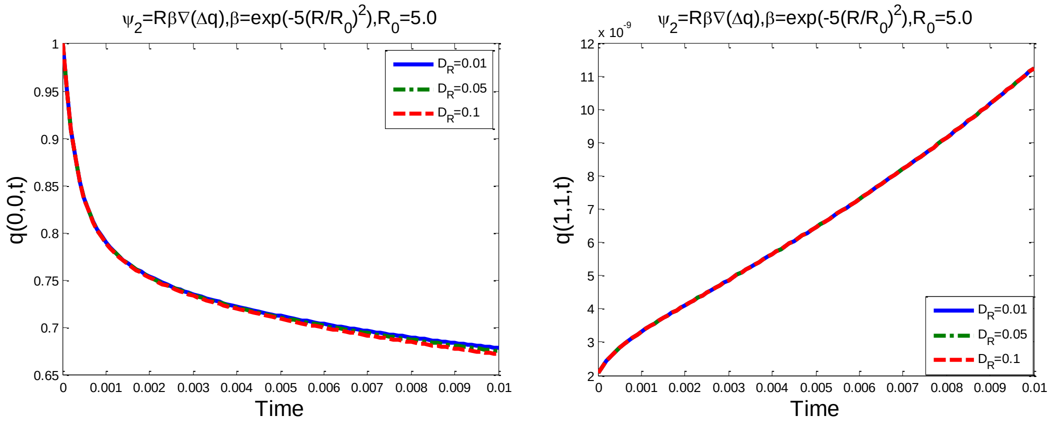


Fig.5.20a Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending diffusion law, for $\boldsymbol{\Psi}_2^{(1)}$ with $D_R = 0.01, 0.05, 0.1, \alpha = 5$

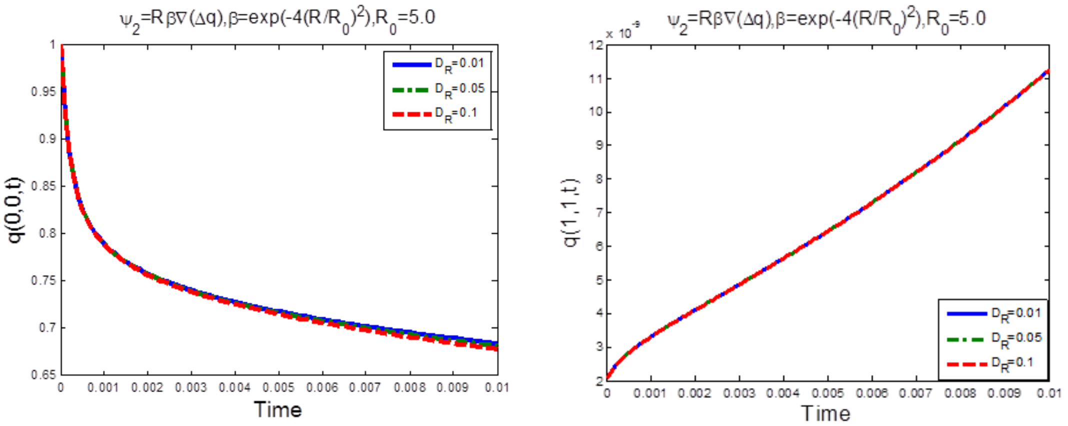


Fig.5.20b Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending diffusion law, for $\mathbf{\Psi}_2^{(1)}$ with $D_R = 0.01, 0.05, 0.1, \alpha = 4$

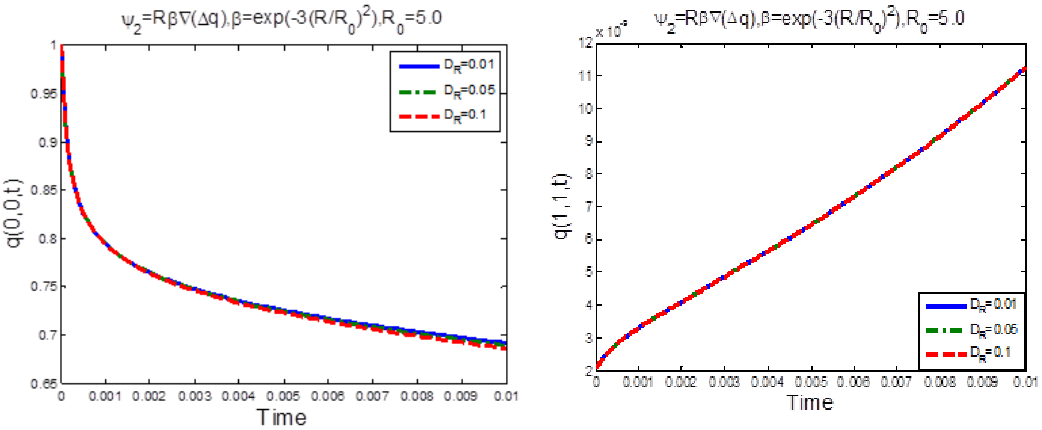


Fig.5.20c Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending diffusion law, for $\mathbf{\Psi}_2^{(1)}$ with $D_R = 0.01, 0.05, 0.1, \alpha = 3$

It is remarkable that for the first class secondary flux potential there is no rising tendency at the central point q(0,0,t) opposing the solution obtained with the second and third classes secondary flux potentials. This result clearly confirm that the deviation from the classical and expected tendency for the concentration to decrease steadily at [0,0] comes mainly from the perturbation on the primary flux. It was shown that the first class potential defining the secondary flux doesn’t introduces any significant alteration on the variables associated to the primary flux.

The influence of α in the exponential law relating β and R is moderate and as expected larger values of α introduce delay in the process. This is apparent by comparing the solutions displayed in the Fig.5.20,a,b,c for t=0.01. The influence of the diffusion coefficient varying in the range, $(0.1{,}0.01)$ doesn't introduce any significant modification on the solution.

Consider now the solution for the case where the second class secondary flux potential is taken.

$$\mathbf{\Psi}_2^{(2)} = R(x,y,t)\nabla(\beta\Delta q(x,y,t))$$

The differential equation system is now:

$$\begin{aligned} \frac{\partial q}{\partial t} &= \nabla\cdot(\beta D\nabla q) - \nabla\cdot(R(1-\beta)\nabla(\beta\Delta q)) \\ \frac{\partial R}{\partial t} &= D_R\Delta R \end{aligned} \tag{5.3}$$

As shown in the Fig.5.21a,b,c the influence of the coupling effect given by the system (5.3) is not significant. The influence of the constant α in the exponential relation connecting β and R is more important than the coupling effect at least for the values of D_R adopted here.

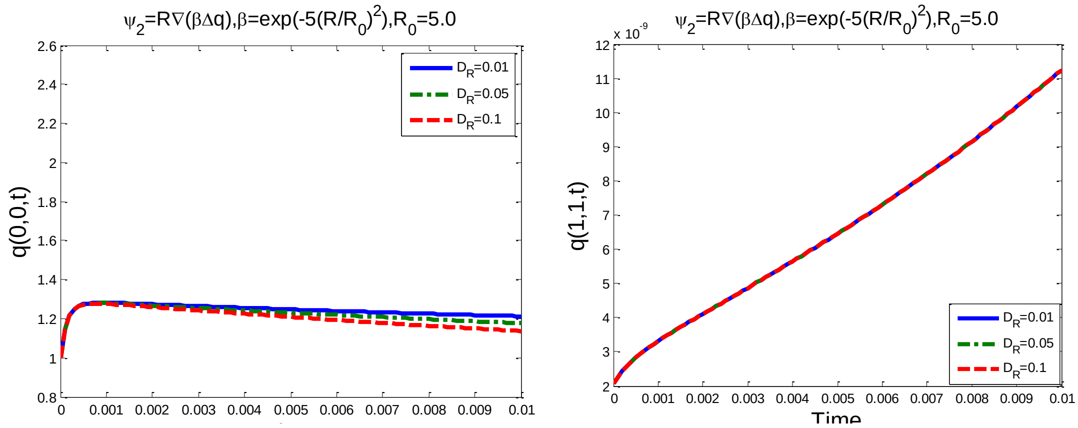


Fig.5.21a Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending diffusion law, for $\mathbf{\Psi}_2^{(2)}$ with $D_R = 0.01, 0.05, 0.1, \alpha = 5$

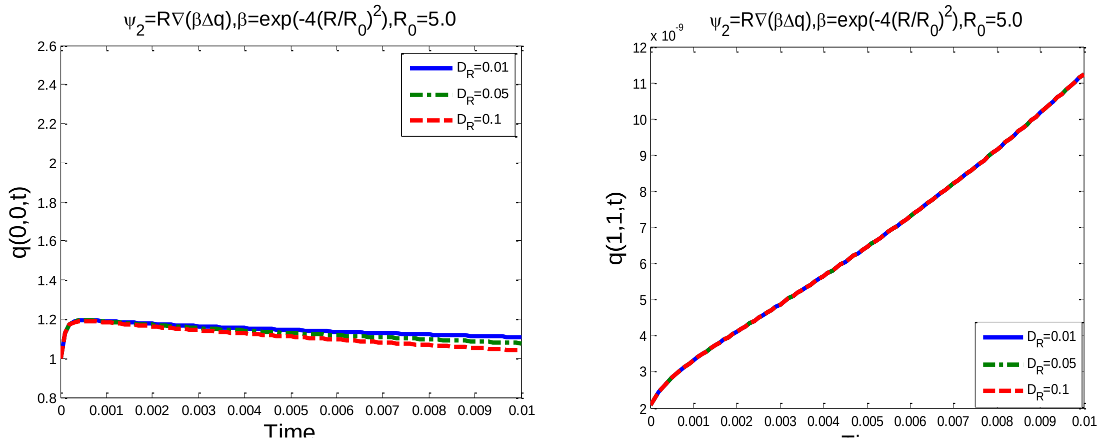


Fig.5.21b Evolution the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending diffusion law, for $\mathbf{\Psi}_2^{(2)}$ with $D_R = 0.01, 0.05, 0.1, \alpha = 4$

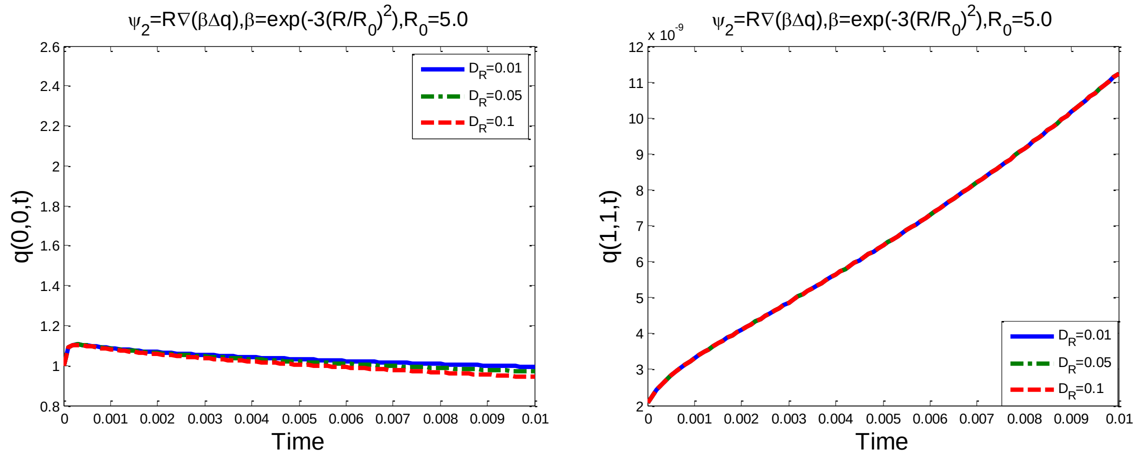


Fig.5.21c Evolution the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending diffusion law, for $\mathbf{\Psi}_2^{(2)}$ with $D_R = 0.01, 0.05, 0.1, \alpha = 3$

Even when compared with the behavior obtained with the reactivity coefficient as a given function of time $R = R_0 \exp\left(-20x^2 - 20y^2 - 10t\right)$ as in the previous section the solution doesn't differ significantly.

Now let us consider the third case corresponding to the third class potential for the secondary flux, that is:

$$\mathbf{\Psi}_2^{(3)} = R(x,y,t)\Delta(\beta\nabla q(x,y,t))$$

The coupled system reads

$$\begin{aligned} \frac{\partial q(x,y,t)}{\partial t} &= \nabla\cdot(\beta D\nabla q(x,y,t)) - \nabla\cdot(R(1-\beta)\Delta(\beta\nabla q(x,y,t))) \\ \frac{\partial R(x,y,t)}{\partial t} &= D_R \Delta R(x,y,t) \end{aligned} \tag{5.4}$$

The solutions are shown in the Fig.5.22a,b,c. Now the behavior of the concentration considering the coupled system (5.4) presents considerable differences as compared with the uncoupled system, that is with R=R(x,y) a time independent coefficient. The influence of D_R is significant. The difference in the solution for R_0=5 at t=0.01considering D_R=0.1 and D_R =0.01 is approximately 78%. The gradient of the time variation of the concentration increases substantially with D_R. The concentrations at t=0.01 for D_R=0.01,0.05 and 0.10 are of the order of 89%, 79% and 70% of the respective maximum values. Increasing values of D_R introduces corresponding larger decreasing rates of the concentration.

It is again shown that the third class flux potential for the secondary flux exerts a strong influence on the behavior of the solution.

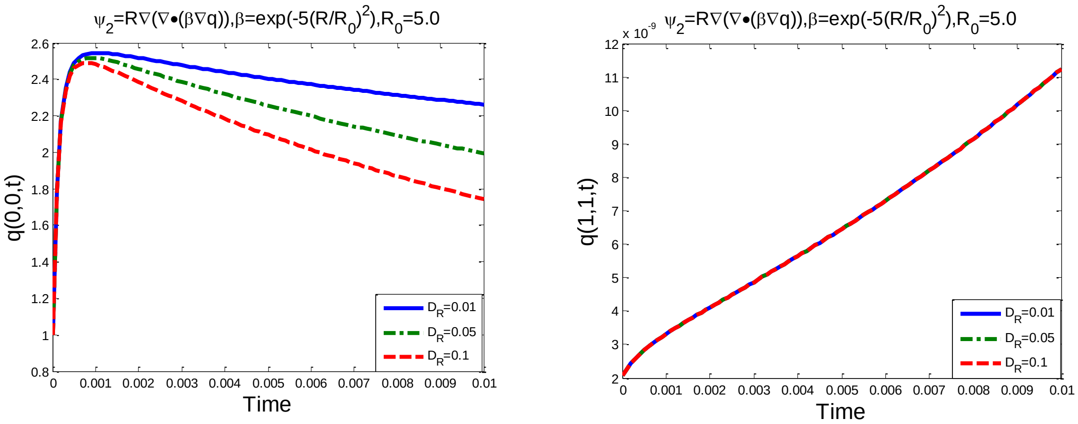


Fig.5.22a Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending diffusion law, for $\mathbf{\Psi}_2^{(3)}$ with $D_R = 0.01, 0.05, 0.1, \alpha = 5$

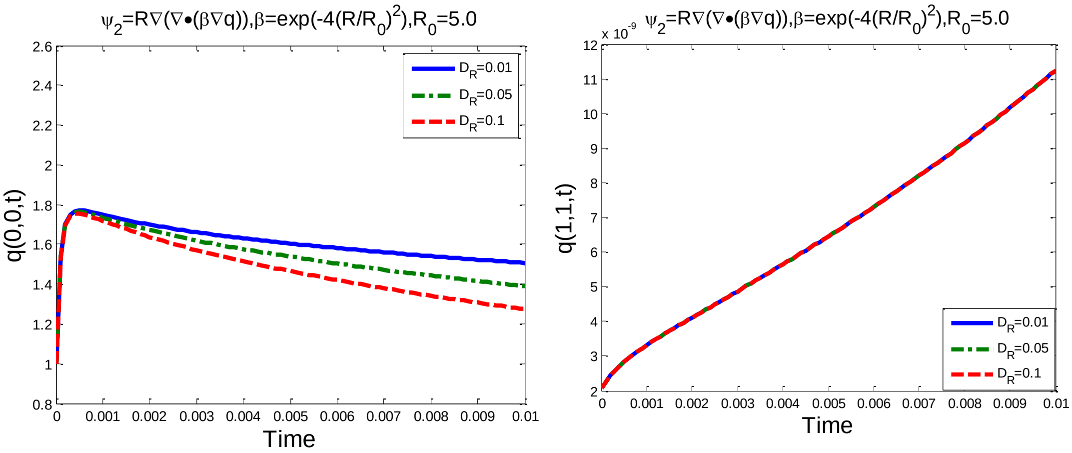


Fig.5.22b Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending diffusion law, for $\mathbf{\Psi}_2^{(3)}$ with $D_R = 0.01, 0.05, 0.1, \alpha = 4$

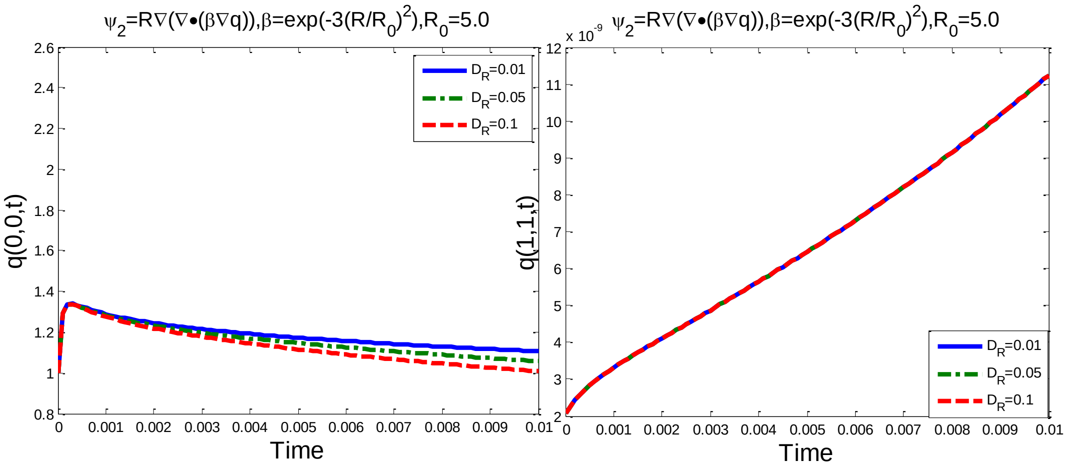


Fig.5.22c Evolution of the concentration profile *q(0,0,t)* and *q(1,1,t),R* depending diffusion law, for $\mathbf{\Psi}_2^{(3)}$ with $D_R = 0.01, 0.05, 0.1, \alpha = 3$

It was shown in this chapter that the definition of the secondary flux potential is critical for the behavior of the solution of the fourth order equation. While the second and third classes definition induce similar behaviors the first class potential leads to a completely different behavior. For the first class potential the primary and secondary fluxes have a weak interaction while for the second and third class flux potentials a strong interaction is developed. It was shown that for appropriate initial and boundary conditions and for particular definition of the reactivity coefficient R(x,y) together with its functional relation with β it is possible for the solution to grow from the initial condition instead of decaying as expected for the classical case. The coupled system with R=R(x,y,t) as an active coefficient spreading according a diffusion law introduces remarkable information only for the case of the third class potential.

The role of the reactivity coefficient as an attractor was confirmed with all the problems solved above. This property suggests strongly that the present approach could be relevant for active biological processes and possibly for social-economics behavior.

The results obtained open a very large window for future research theoretical and applied. The new tool can be explored to improve several cases of diffusion and to model new complex phenomena.

Chapter 6

A hypothesis for the bi-flux process and the time evolution of β in an ideal universe

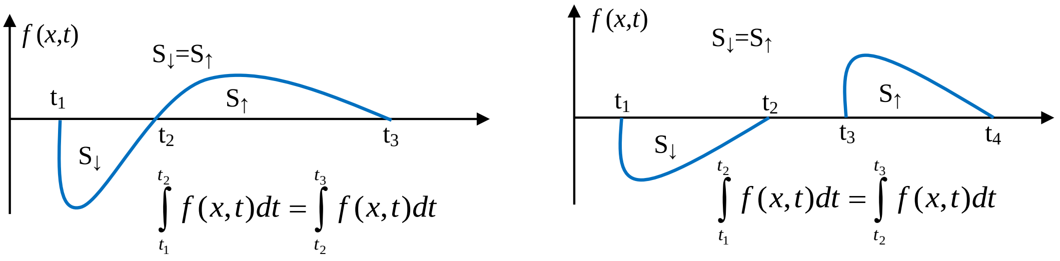
6.1 The hypothesis for retention process

It is not the purpose of this thesis to discuss the physics of the retention process. Nevertheless a suggestion will be briefly presented here. It is based on the interaction among particles that exchange kinetic energy. It is of course an ideal universe. But before entering the possible explanation for the bi-flux theory let us explore briefly other situations that can interfere on the flux, but are quite different from the approach used in this thesis.

Retention processes may be simulated by subtracting and adding equal fractions of particles in a continuous or discontinuous process. This formulation of the problem is equivalent to deal with the classical diffusion equation incorporating a source-sink term. For one dimensional flow and constant diffusion coefficient the new equation reads:

$$\frac{\partial q}{\partial t} = D\frac{\partial^2 q}{\partial x^2} + f\left(x,t\right)$$

The function $f(x,t)$ represents the effect of a source or a sink depending respectively on the plus or minus sign of that term in the differential equation. If $\int_{t_i}^{t_f} f(x,t)dt$ for t_i and t_f covering a sufficient large interval, Fig.6.1, then the above equation can be considered as representing diffusion with temporary retention provided that after a finite time all particles active in the process at $t=0$ are back into the process. This idea fits into several proposals presented in the literature and may work well for particular cases.



(a) (b)

Fig.6.1. Source-sink function simulating temporary retention in a continuous process (a) and discontinuous process (b)

It is not a law properly speaking it is an adjustment factor that assumes energy exchange with the surrounding environment.

On the contrary, the law proposed here keeps the particles all the time in the system distributed in two concomitant fluxes with different flux rate groups that may represent “temporary retention” without exchange of energy with the surroundings. The underlying idea in the theory presented here is the energy distribution associated with the linear momentum and angular momentum. A particle is said to be blocked whenever its angular momentum prevails over the linear momentum. Fig. 6.2(a) illustrates the motion distribution assumed here. It is important to remark that in our model all particles are continuously participating in the evolution phenomenon, and what we call “trapped” or “blocked “ particles are in reality subjected to a slow motion, as slow as we wish, in the same direction of the main flux or in the counter-flux direction.

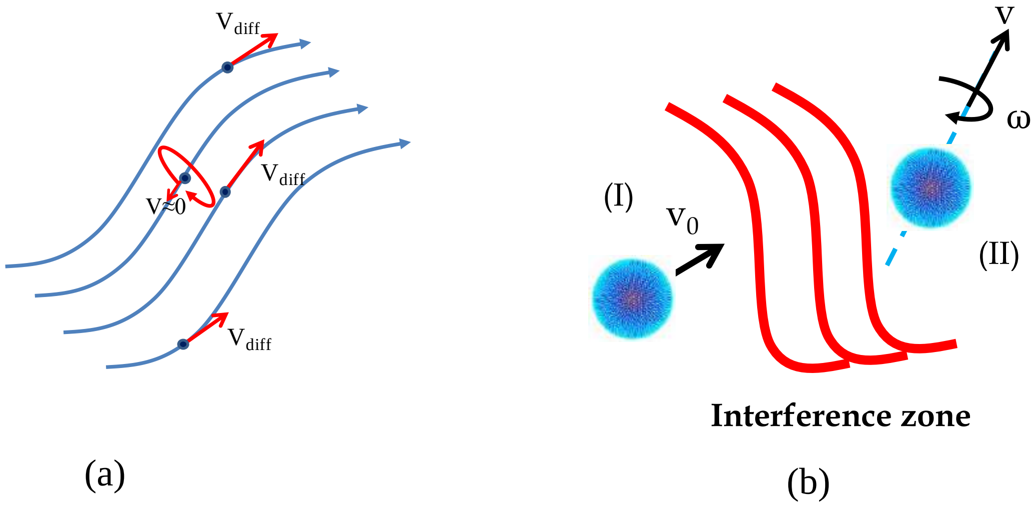
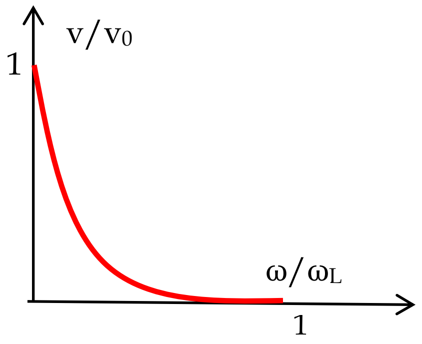


Fig.6.2 (a) Illustration of particles moving along the flow trajectory, diffusing particles, and delayed particles. (b) Interaction in an interference zone with energy conservation. (I) State before interference (II) State after interference.

The result of the interaction among particles changes the energy state of the particles introducing several microstates. In the present approach the several states are reduced to two fundamental states. Assuming energy conservation a given particle with mas "m" and moment of inertia "I" is initially moving without rotation with velocity "v_0". The kinetic energy is then:

$$E_0 = \frac{1}{2} m v_0^2$$



After interacting with other particles the new kinematical state is $[v, \omega]$. With energy conservation, under very small temperature changes, we may write:

$$m v_0^2 = m v^2 + m \lambda^2 \omega^2$$, where we put $I = m\lambda^2$

Now let us assume that there is a limit ω_L for the angular velocity such that as $v \to 0$, $\omega \to \omega_L$. Assume that (Fig.6.3):

$$\frac{v^2}{v_0^2} = \exp\left(-\frac{\omega^2/\omega_L^2}{1-\omega^2/\omega_L^2}\right)$$

That is when $z = \omega/\omega_L \to 1$ than $v \to 0$ and all the kinetic energy is transferred to the rotational energy. The system is stand still after all particles assume the rotational state. If $\omega = 0$ the system is in a pure diffusion state. Substituting the above relation in the energy conservation principle we obtain:

$$\frac{E_\omega}{E_0} = \frac{1}{z^2}\left\{1-\exp\left(-\frac{z^2}{1-z}\right)\right\} \quad \text{where,} \quad z = \omega/\omega_L$$

6.2.A law for the variation of β with time

6.2.1 The energy partition

In the previous section we introduced briefly some comments on the energy partition between particles belonging to the fluxes $\mathbf{\Psi}_1$ and $\mathbf{\Psi}_2$, here we will develop this idea. Let us explain first what we understand by excitation state. Consider a particle moving with linear velocity **v** and rotating with angular velocity **ω**. The linear momentum **p** and the angular momentum **L** are given respectively by $\mathbf{p} = m\mathbf{v}$ and $\mathbf{L} = m\bar{d}^2\boldsymbol{\omega}$ where *m* is the mass of the particle and $\bar{d}$ is the effective gyration radius. Let us call active energy or translational energy the kinetic energy associated to the linear momentum. That is if **p** is the linear momentum of a given particle P, its active energy is $\mathrm{e_p} = \mathbf{p}^2/2m$ where *m* is the mass of the particle. The rotational energy e_ω corresponds to the kinetic energy generated by the angular momentum **L**, that is $\mathrm{e}_\omega = \mathbf{L}^2/2m\bar{d}^2$. Any particle may be moving with linear momentum **p** and angular momentum **L**, the total energy e however remains constant, $\mathrm{e} = \mathrm{e_p} + \mathrm{e}_\omega =$ constant. We will consider that energy conservation is true for all particles under consideration, that is, the system is conservative.

Now suppose that we have a system consisting of N particles where the particles are divided into two subsets, $N_1=\beta N$ and $N_2=(1-\beta)N$. The energy density or specific energy (energy/volume) corresponding to N_1 and N_2 are respectively, $\mathrm{E}_1 = \beta\mathbf{\Psi}_1^2/2q$ and

$\mathrm{E}_2 = (1-\beta)\left(\mathbf{\Psi}_2^2/2q + \mathrm{E}_\omega(\beta)\right)$. Therefore we assume that all particles excited in the state E_1 do not rotate, all kinetic energy is stored as active energy, while the kinetic energy corresponding to the state E_2 is stored as active energy and rotational energy $\mathrm{E}_\omega(\beta)$ as well. Note that since the system is conservative we have $\mathrm{E}=\mathrm{E}_1+\mathrm{E}_2 \rightarrow$ constant. We may consider the rotational energy as a hidden form of energy and the parameter $(1-\beta)$ as the probability of occurrence of rotational energy. Indeed for pure Fickian processes $(1-\beta)=0$ there is no rotational energy in the system, $\mathrm{E}_\omega(1)=0$, and for $(1-\beta)=1$ all energy is stored as rotational energy $\mathrm{E}_\omega(0)=\mathrm{E}$. Let us call $\mathrm{E}_\omega(0)=\mathrm{E}_\omega^*$. Recall that if $\beta=0$ then $\mathbf{\Psi}_2 = 0$. The contribution of the rotational energy of all particles to E_2 is wrapped up in the energy density term $\mathrm{E}_\omega(\beta)$.

Suppose now that we are dealing with a dynamic system, that is, there is a continuous internal energy exchange in the system $\mathrm{E}_1 \leftrightarrow \mathrm{E}_2$. The energy distribution is clearly controlled by the parameter β. Therefore to perform the analysis of a dynamical diffusion process as exposed above in an isotropic medium it suffices to assume the fraction $\beta(t)$ varying in time and the diffusing particles distributed between two time dependent energy states. Note that the Eq.2.9 still holds for $\beta=\beta(\mathrm{t})$. Recalling Eq.2.9

$$\frac{\partial q}{\partial t} = \beta D \frac{\partial^2 q}{\partial x^2} - \beta(1-\beta) R \frac{\partial^4 q}{\partial x^4}$$

As suggested above, in diffusion processes, particles collide continuously exchanging linear momentum and angular momentum. In principle at each collision active energy may be converted into rotational energy and the other way around. In our particular universe we will consider two distinct and opposite phase states. The phase state S_1 is such that active energy is always converted into rotational energy while in the phase state S_2 rotational energy is always converted into active energy. Let us introduce the following rules that apply in our particular universe (Rhee *et al.*, 2012)

1) In an isolated system the total kinetic energy remains constant therefore $\mathrm{E}_1 + \mathrm{E}_2 = \beta \mathbf{\Psi}_1^2/2q + (1-\beta)\left(\mathbf{\Psi}_2^2/2q + \mathrm{E}_\omega(\beta)\right) = \text{constant}$ for all t.

2) In an isolated system subjected to the phase state S_1 the rotational energy increases and the active energy decreases continuously. Therefore in an isolated system $\mathrm{S}_1 \lim_{t\to\infty} \mathrm{E}_1 \to 0$ and $\lim_{t\to\infty} \mathrm{E}_2 \to \lim_{t\to\infty} \mathrm{E}_\omega(\beta)$. This means that $\beta = \beta(\mathrm{t})$ is a function of time and $\beta(\mathrm{t}) \rightarrow 0$ as $\mathrm{t} \rightarrow \infty$.

3) In an isolated system subjected to the phase state S_2 the active energy increases and the rotational energy decreases continuously. Therefore in an isolated

system $S_2 \lim_{t\to\infty} E_1 \to E$ and $\lim_{t\to\infty} E_{\omega}(\beta) \to 0$. This means that $\beta = \beta(t)$ is a function of time and $\beta(t)\to 1$ as $t\to\infty$.

According to the hypothesis introduced above, a complex diffusion process consisting of a very large number of micro-states is reduced to two fundamental non-stationary states governed by a primary volumetric flow rate $\mathbf{\Psi}_1$ and a secondary volumetric flow rate $\mathbf{\Psi}_2$ that represent the overall average of micro-states (see appendix). If the system is in the phase state S_1 as time increases it tends to the stationary state E_{ω} .For a system in the phase state S_2 all particles will be excited in the energy state E_1 after a sufficient long time. Now as $\beta= \beta(t)$ is function of time, as time varies the parameter $0<\beta<1$ covers the whole energy distribution spectrum for both cases

6.2.2 Isolated system in the phase state S_1.

Consider now a one-dimensional problem defined in some interval $x \in [a,b]$. Let us assume that the distribution of particles in states E_1 and E_2 is independent of x but may vary in time. The system is isolated and according to the model exposed in the previous section the system tends to rest meaning that the total active energy tends to zero as $t\to\infty$. Since the system is isotropic the linear momentum tends uniformly to zero for all x as $t\to\infty$, that is $\lim_{t\to\infty}\mathbf{p}(x,t)\to 0$. Consequently $\lim_{t\to\infty}\beta(x,t)\to 0$.Under these conditions let us find an expression for the decay of the fraction β as function of time. Clearly the probability of interaction among particles is proportional to β inducing a reduction of particles in state E_1. That is, the variation $\delta\beta$ is proportional to β. This means that the change of the excitation state, active energy into rotational energy ($\mathbf{p}\to\mathbf{L}$), is more intense when the number of particles in state E_1 is large $\beta>>0$.

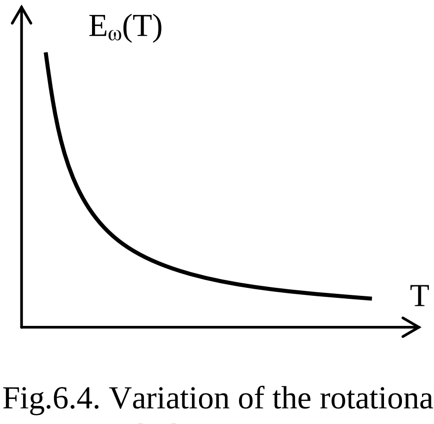


Fig.6.4. Variation of the rotational energy with the parameter T

Besides the probability of interaction among particles the rate of the variation $\delta\beta$ depends on the energy contained in the state E_1 or alternatively on complementary state E_2. Let T(t) be the variable that measures the active energy contained in the state E_1. It might be an indirect measure of the linear momentum of the particles in the system. Since the system is isolated and the total energy is constant, T(t) is also an indirect measure of the rotational energy. Let $E_\omega(T)$ represent the rotational energy. Clearly $E_\omega(T)$ is decreasing functions of T (Fig.6.4).

At very large energy levels T>>0 the rate of variation of the rotational energy $E_\omega(T)$ with respect to the energy parameter T is low. But for T small big variations of the angular momentum occurs for relatively low decrease of the energy parameter T. Therefore it is reasonable to assume as a first approximation:

$$E_\omega(T) = F\left(\frac{T_0}{T}\right) \tag{6.1}$$

The variation $\delta\beta$ depends therefore on two determinant parameters:

1. The fraction of particles in the state E_ω given by β.
2. The variation of the rotational energy given by $-\delta(E_\omega(T))$. The negative sign meaning that β decreases as E_ω increases.

With the hypotheses above it is possible to define the variation of β:

$$\delta\beta = \beta\frac{(-\delta E_\omega)}{K_0}$$

where K_0 is a given energy parameter. Now with the Eq6.1 we may write:

$$\delta E_\omega = -\frac{T_0}{T^2}\frac{dF}{du}\delta T$$

where $u=T_0/T$. Introducing the expression above in the equation for $\delta\beta$ we get:

$$\delta\beta = \beta\frac{1}{K_0}\frac{T_0}{T^2}\frac{dF}{du}\delta(T)$$

After integration:

$$\beta = \exp\left(\int\left(\frac{T_0}{K_0}\frac{1}{T}F_u\right)\frac{1}{T}\frac{\partial T}{\partial t}dt\right) \tag{6.2}$$

Where $F_u = dF/du$. Now define:

$$S_\omega = \frac{1}{T}F_u$$

The function S_ω may be understood as the entropy referring to the present theory applied to isolated systems. Introducing this expression in Eq.6.2 we get:

$$\beta = \exp\left(\frac{T_0}{K_0} \int S_\omega \frac{\partial}{\partial t} \ln T dt \right)$$

With:

$$\frac{\partial}{\partial t} \ln T = g(S_\omega) \qquad \text{and} \qquad \frac{K_0}{T_0} = S_0$$

We finally obtain:

$$\beta = \exp\left(\int \frac{S_\omega}{S_0} g(S_\omega) dt \right)$$

Assuming now the simplest expression for the energy $E_\omega(T)$, that is, according to Eq.6.1 $E_\omega(T)=K_1(T_0/T)$, $F_u = K_1$ and with Eq.6.2 it is readily obtained:

$$\beta = \exp\left(-\frac{1}{S_0} \int \frac{\partial S_\omega}{\partial t} dt \right) \tag{6.3a}$$

That after integration gives the general expression:

$$\beta = \exp\left[-\frac{S_\omega(t)}{S_0} \right] \tag{6.3b}$$

Therefore $S_\omega = -S_0 \ln \beta$ or $S_\omega = S_0 \ln(N_1/N)$. We will call the variable S_ω as *ω-entropy*. It is a measure of the relative organization of particles in two states S_1 and S_2. S_ω indicates the equivalent number of particles excited in a pure rotational energy state or likewise at rest, meaning x_i = constant (i=1,2,3), in a given inertial frame. That is, as $S_\omega \to \infty$ or similarly $\beta \to 0$ the relative distances among all particles tend to remain fixed and the system approaches a stationary state. If it would be only possible to measure the active energy, then for very large values of S_ω an external observer would come to the conclusion that the system is inactive or “dead”. Maybe only the mass could be detected and the rotational energy stored in the system would be hidden, it would be a kind of “dark energy”.

Since the active energy for this system is a decreasing function of time and the variation rate of change is inversely proportional to the active energy level it is reasonable to admit that $\partial S_\omega / \partial t = U_0 t$ where U_0 is a constant of the system. From which follows $S_\omega = U_0 t^2/2$, and finally:

$$\beta = \exp\left(-t^2/\tau_0^2 \right)$$

where, $U_0/2S_0 = 1/\tau_0^2$

6.2.3 Isolated system in the phase state S$_2$.

This system, sustained by the phase state S$_2$ has the opposite property of the previous one, that is, the collision between two particles always transforms angular momentum into linear momentum but not the other way around. This means that ultimately the initial rotational energy will be totally converted into active energy. Suppose that initially the total energy in the system is stored under the form of rotational energy E_ω^*.That is, the fraction β increases gradually from $\beta(0)$ =0 up to $\beta(t^*)$ =1 which is the maximum possible value. We want to analyze the behavior of the phase change up to t=t*.

The evolution of the fraction β, with a first approximation for the energy function, is given by the expression 6.3-a derived before with the exponent multiplied by –1. Indeed we have now $S_\omega(0) > S_\omega(t)$ for all t>0 and consequently $\delta\beta = \beta(\delta\mathrm{E}_\omega)$ which explains the change in sign. Now the simplest approximation for the variation of the ω-entropy coherent with the variation for S$_1$is given by $\partial S_\omega/\partial t = -\hat{U}_0 t^{-3}$. Note that now the ω-entropy is a decreasing function of time given by $S_\omega = \hat{U}_0 t^{-2}/2$. Therefore we may write from 6.3-b:

$$\beta = \exp\left(-\tau_0^2/t^2\right)$$

Where, $\hat{U}_0/2S_0 = \tau_0^2$. Note that under the above assumptions t* →∞.

This case, the S$_2$ phase state, is more complex than the first one S$_1$. The transfer of rotational energy to active energy is not so easy and would require an external potential field to initiate and probably to sustain the process. So the present approach is only a first approximation. Note that the phase S$_1$ is related to extinction while S$_2$ is related to creation which is always more difficult to be analyzed and simulated.

6.2.4 Selected examples.

Consider now the bi-flux diffusion process defined on the interval $[-1,1]$ for an isotropic supporting medium. If the fraction β is function of time the governing equation 6.3 is written as :

$$\frac{\partial q}{\partial t} = \beta(t) D \frac{\partial^2 q}{\partial x^2} - (1-\beta(t))\beta(t) R \frac{\partial^4 q}{\partial x^4}$$

Assume that the primary and secondary fluxes vanish at the boundaries, x=1 and x=−1. The boundary conditions therefore read:

$$\left.\frac{\partial q}{\partial x}\right|_{x=\pm 1} = 0 \text{ and } \left.\frac{\partial^3 q}{\partial x^3}\right|_{x=\pm 1} = 0$$

Let the initial condition be:

$$q(x,0) = 0.25(1+\cos(\pi x)) \qquad -1 \le x \le 1$$

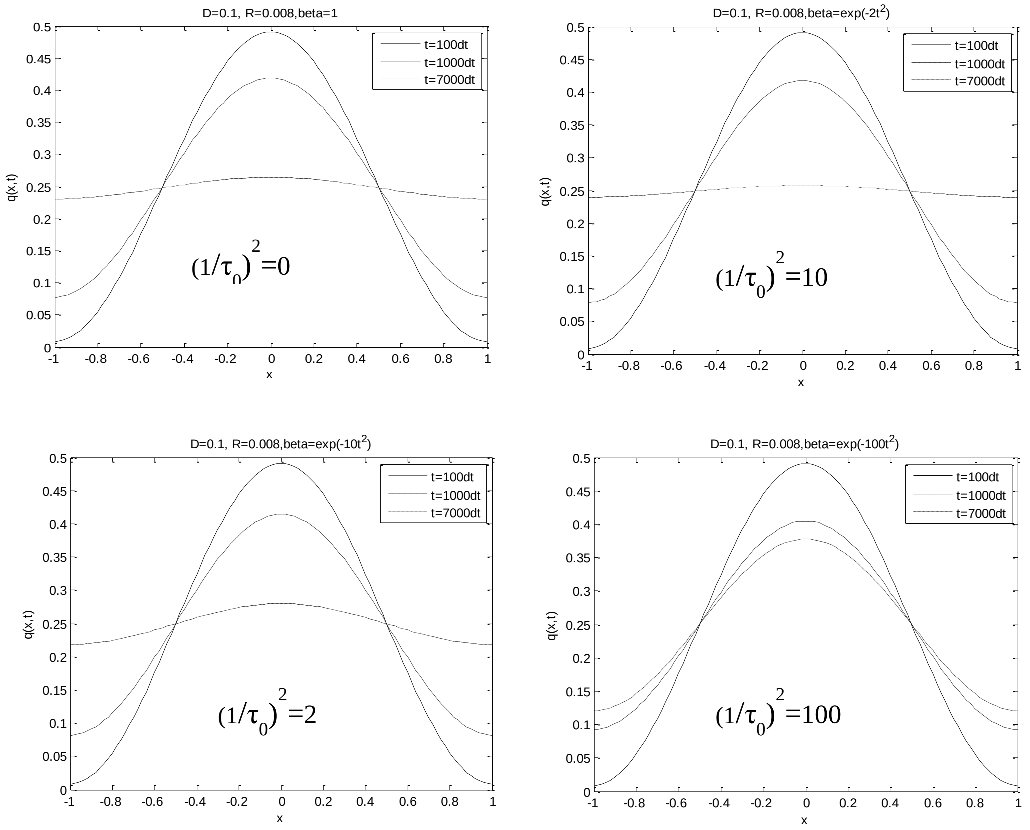


Fig.6.5. Evolution of the concentration profile in an isolated system. Energy is being transferred from S_1 to S_2 at different rates $1/\tau_0$. For $1/\tau_0=0$, $\beta=1$, Fickian

Suppose that initially, *t*=0, the system is subjected to a pure Fickian process, that is, only the primary flux exists. Since there is no energy exchange with the surroundings, according to our hypothesis, the primary flux will decrease and the secondary flux will increase as time increases. Energy is continuously transferred from the primary flux to the secondary flux. Now for an isolated system starting with a full Fickian diffusion regime, that is $\beta(0)=1$ Eq.4.3b prevails, that is:

$$\beta = \exp\left(-t/\tau_0\right)^2$$

The diffusion and reactivity coefficients are taken D=0.1 and R= 0.008 respectively. Fig.6.5 shows the concentration profile for different values of the parameter τ_0. For values relatively high, $\tau_0 = 1/\sqrt{2}$ the freezing process is low and stabilizes close to the uniform solution, that is, $\underset{\lim t\to\infty}{q(x,t) = const.}$. Note that both fluxes are blocked at the ends $x=+1$ and $x=-1$and the diffusion process imposes $q(x,t)$ constant as $t\to\infty$. As the value of τ_0 decreases the freezing progression is quicker. For τ_0=0,1 there is almost no time to initiate the diffusion process and the density distribution after a sufficient long time is almost the same as the initial conditions. Fig.6.6 shows the time variation of the concentration at x-0. For values of τ_0 less than 0.1 the steady state is reached very quickly and the final concentration distribution remain close to the initial condition. Since β goes to zero as time increases in all the cases the primary flux will vanish and the concentration profile $q(x,t)$ will freeze for very large t. It is interesting to observe that the gradient of the concentration alone is not determinant to trigger the diffusion process, it is also necessary the presence of particles in state E_1. If the system has attained the limiting state $E_2=E^*_\omega$, than there is no flow irrespective of the concentration profile.

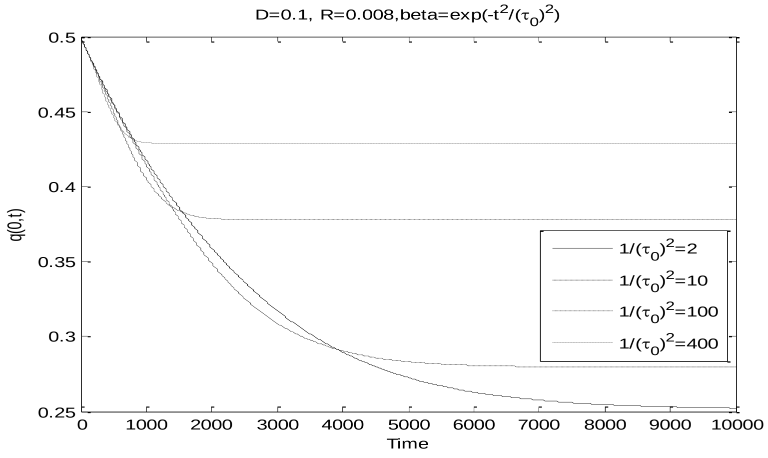


Fig.6.6. Evolution in time of the concentration at x=0 for different values of τ_0.

Now consider the second case where the system belongs to the phase state S_2 initially free of active energy but subjected to a continuous influx of active energy at the expense of rotational energy. Let the boundary conditions be the same as before and take the following initial condition:

$$q(x,0) = 0.25(2 - \cos(\pi x))$$

Initially the system is inactive; there is no flux at all, neither primary nor secondary. Now, since rotational energy is being continuously transformed into active energy the fraction β will steadily increase. The law governing this behavior is given by $\beta = \exp\left(-\tau_0^{\,2}/t^2\right)$ as explained before. Fig.6.7 shows the evolution of the bi-flux process for different values of τ_0. For very low energy transfer rates, τ_0 large, the system tends to equilibrium very slowly. For low values of τ_0 the system behaves almost like a pure Fickian process. Note that since there is no flow at the boundaries the system tends to the steady state with the concentration $q(x,t)$ constant along the domain $[-1,1]$.

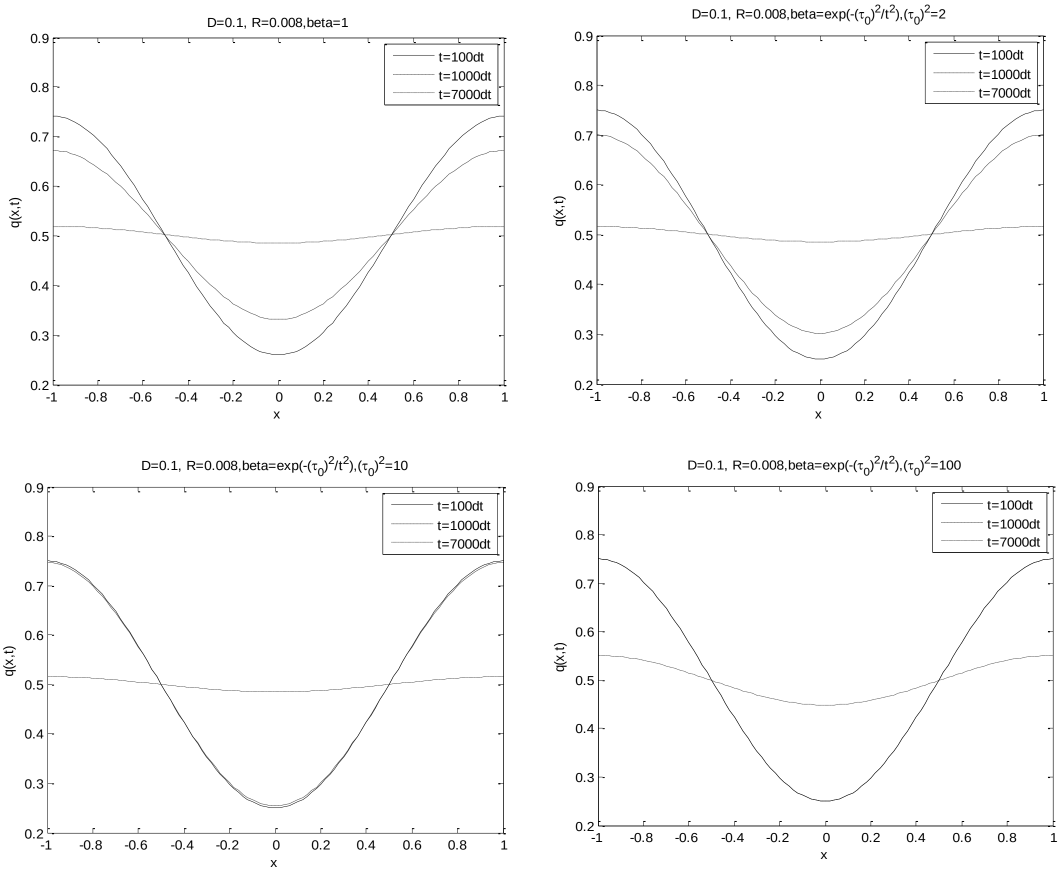


Fig.6.7. Evolution of the concentration profile $q(x,t)$ for a non-conservative system. Energy is being continuously transferred to the system at different rates τ_0. For $\tau_0=0$, $\beta=1$, Fickian diffusion.

The variation of the concentration with time, $q(0,t)$, at x=0, for various values of τ_0 is shown in Fig.6.7. Here the fraction β of particles belonging to the Fickian diffusion increases steadily in time. Therefore eventually the final concentration profile will coincide with the expected profile for a Fickian process that is a uniform distribution on the region -1<x<1. The evolution of $q(0,t)$ shown in the Fig.6.8 shows clearly this tendency.

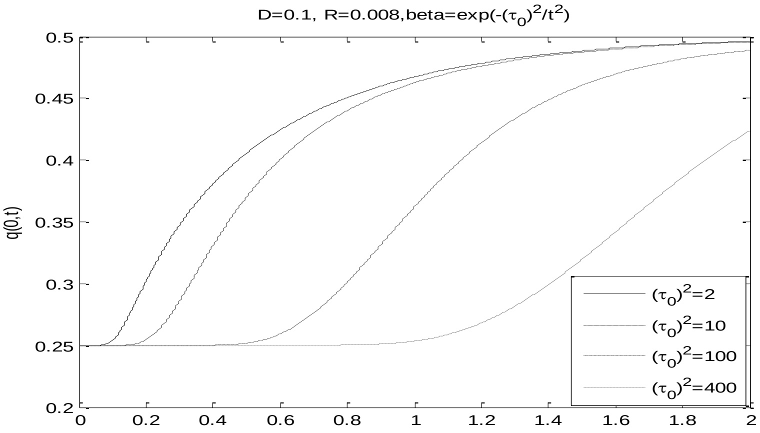


Fig.6.8. Evolution in time of the concentration at x=0 for different values of τ_0

The hypothesis advanced above considering the effect of rotation has been raised by some authors. Their approaches are rather complex and might be coupled to the bi-flux assumption with a possible simplification of the diffusion process. (Murray, 2008)

Chapter 7

Two examples of the influence of nonlinear source and sink

In this chapter it will be shown the effect of the presence of non-linear source and sink on the solution of the bi-flux equation. Two types of classical equations will be used in order to compare the solution obtained with the new approach with classical solutions. The purpose of this final section is simply to compare some typical cases. A detailed study of the existence, uniqueness and stability conditions is not included in the purpose of this thesis. It will be however shown that there can be interesting effects introduced by the bi-flux equation particularly referring to the regularity of some solutions. This chapter as the others focuses on the numerical solutions of some specific cases and tries to highlight the most critical differences with respect to the classical solutions. Two types of equations were selected: the Fisher-Kolmogorov extended equation and the Gray-Scott equation. Both represent the model of important events in chemical and biological sciences (Araujo, 2014; Dee,1988; Peletier, 1996, 1997).

7.1. The Fisher-Kolmogorov equation.

The Fisher Kolmogorov equation was developed independently by Fisher and Kolmogorov. One of the important motivations was the modeling of genetic modification. The particular property of this equation is the generation of travelling waves that are adequate to represent the genetic modification in a given population (Fisher, 1937). We will not go into this discussion but will be restricted to the comparison of the solutions given by the classical approach and the bi-flux approach.

The classical Fisher Kolmogorov equation reads:

$$\frac{\partial q}{\partial t} = D\frac{\partial^2 q}{\partial x^2} + \gamma q(1-q) \quad \text{with } 0<q<1$$

The stationary equilibrium solutions is stable for $q = 1$ and unstable for $q = 0$. We will discuss the extended Fisher Kolmogorov equation of the form:

$$\frac{\partial q}{\partial t}=D\frac{\partial^2 q}{\partial x^2}+\gamma q\left(1-q^2\right) \qquad \text{with } 0<q<1 \tag{7.1}$$

This equation is similar to the previous one with stable solutions for $q=0$ and unstable solutions for x=±1. The solution for a simple case of (7.1) will be compared with the corresponding bi-flux equation:

$$\frac{\partial q}{\partial t}=D\beta\frac{\partial^2 q}{\partial x^2}-R\beta(1-\beta)\frac{\partial^4 q}{\partial x^4}+\gamma q\left(1-q^2\right) \tag{7.2}$$

Let us solve the problem in the interval [-1,1] and take the following values for the parameters:

D=0.02, β=0.5, R=0.04, γ=1

The initial condition is $q(x,0)=\exp\left(-10x^2\right)$ and the boundary conditions:

$$\partial q(-1,t)/\partial x=\partial q(1,t)/\partial x=0 \quad \text{and} \quad \partial^3 q(-1,t)/\partial x^2=\partial^3 q(1,t)/\partial x^2=0$$

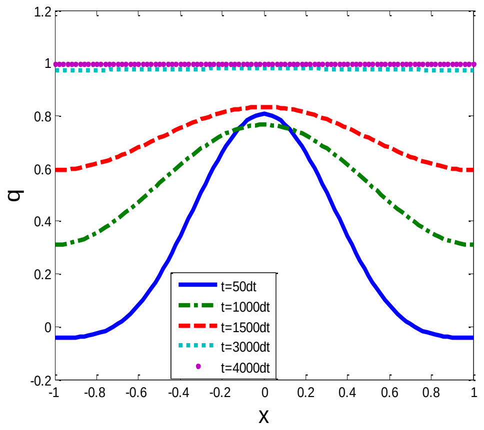


Fig.7.1a F-K equation with bi-flux

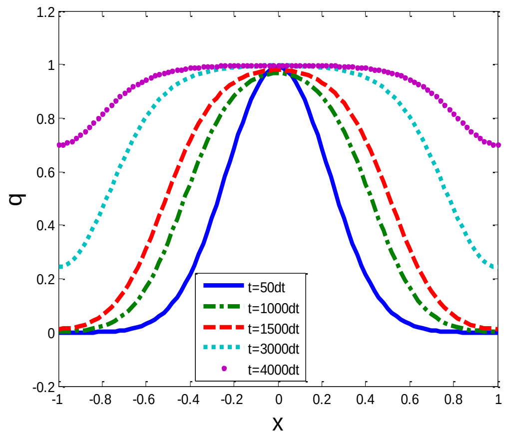


Fig.7.1b F-K equation

Figures 7.1a and 7.1b represent the evolution of the bi-flux theory and the classical theory. The general aspect doesn't differ essentially for the two approaches. The solution, for both cases, tends to the stable condition q(x,∞)=1 as estimated by the theory. In this aspect the only difference is the speed of convergence much higher for the bi-flux approach. Again, as expected, negative values appears for the bi-flux solution close to the ends. This is a typical behavior that has been confirmed by the solution obtained by Danumjava *et al.* (2006) and Khiari *et al.* (2011) that uses also a fourth order partial differential equation but with no particle distribution in two distinct energy states given by the fractions β and (1- β) as in the present theory.

Now in order to test the convergence of the method the analytical solution for a given problem was compared with the numerical solution. Consider the equation:

$$\frac{\partial q(x,t)}{\partial t} = \beta D \frac{\partial^2 q(x,t)}{\partial x^2} - \beta(1-\beta)R\frac{\partial^4 q(x,t)}{\partial x^4} + q - q^3 + g(x,t)$$

where

$$g(x,t) = \cos(2\pi x)e^{-t}\left(16\beta(1-\beta)R\pi^4 + \beta D\pi^2 - 2 + \cos^2(2\pi)e^{-2t}\right)$$

The initial condition is defined as $q(x,0) = \cos(2\pi x)$, and the boundary condition are given by: $\partial q(0,t)/\partial x = \partial q(1,t)/\partial x = 0$, $\partial^3 q(0,t)/\partial x^2 = \partial^3 q(1,t)/\partial x^2 = 0$. The parameters are: $D = 2.0, \beta = 0.5, R = 0.4$ .The term $g(x,t)$ was introduced such that the analytical solution would be of the form:

$$q(x,t) = \cos(2\pi x)e^{-t}$$

Now take $\partial^2 q(x,t)/\partial x^2 = v(x,t)$ to define the system two of second order equations:

$$\partial^2 q(x,t)/\partial x^2 = v(x,t)$$

$$\frac{\partial q(x,t)}{\partial t} = \beta D \frac{\partial^2 q(x,t)}{\partial x^2} - \beta(1-\beta)R\frac{\partial^2 v(x,t)}{\partial x^2} + q - q^3 + g(x,t)$$

The error of the numerical solution using the non-linear Galerkin method (Marion and Temam, 1989, 1990, 1995; Nabh *et al.*, 1996; Dubois *et al.*,, 1998, 1999, 2004; Dettori *et al.*,, 1995; Laminie *et al.*,,1993; García-Archilla *et al.*,, 1995) compared with the exact solution is given in the table 7.1. The element size is given by $h = 1/N$ in the table, with N representing the number of elements. The time step $\Delta t = 1/h^2$.

Table 7.1 CPU time, error and order of accuracy for q in F-K model with bi-flux model under nonlinear Galerkin method

N	h	Δt	CPU(s)	L_∞ for q	Order	L_2 for q	Order
5	0.2	0.04	0.042	2.70e(-3)	----	2.20e(-3)	----
10	0.1	0.01	0.083	8.39e(-4)	1.69	6.51e(-4)	1.76
20	0.05	0.0025	0.426	2.20e(-4)	1.93	1.63e(-4)	2.00
40	0.025	6.25e(-4)	3.212	5.56e(-5)	1.98	4.04e(-5)	2.01
80	0.0125	1.56e(-4)	26.26	1.40e(-5)	1.99	1.00e(-5)	2.01
160	0.0063	3.91e(-5)	202.08	3.49e(-6)	2.00	2.49e(-6)	2.01

Final time T=1.0

It is seen that the method converges exponentially with decreasing size of the elements. The CPU time however increases also exponentially with the number of elements.

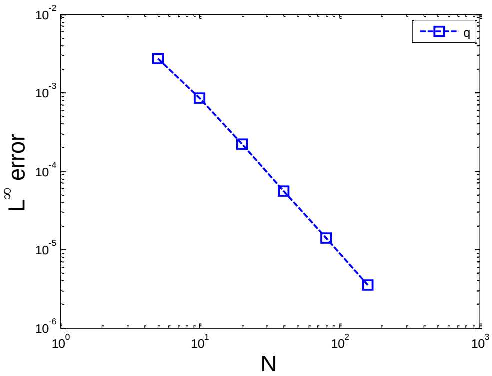


Fig.7.2a. Cell N vs $\alpha=3$error

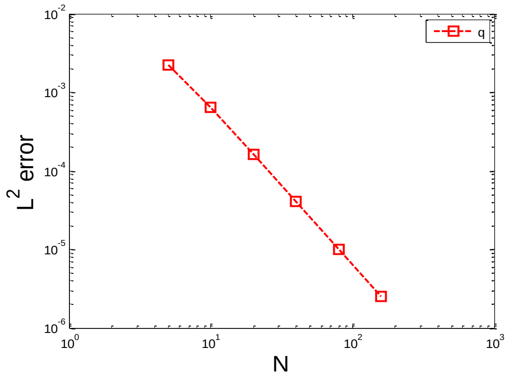


Fig.7.2b. Cell N vs L^∞ error

The Fig.7.2a,b represent the errors in L^∞ an L^2 as functions of the number of elements N. The convergence for both norms is quite satisfactory. Although this is a particular solution the results indicate that the numerical method works well.

7.2. The Gray-Scott equations

The reaction process of two chemicals in which one of them is catalytic compound can be modeled by the Gray-Scott equations. We will consider the one dimensional Gray-Scott model, in which self-replicating patterns have been observed (Pearson, 1993; Lee *et al.* 1994). There are several approaches to deal with the Gray-Scott equations since the solutions can belong to different classes. Travelling waves can be generated in one dimensional domain with appropriated initial conditions, standing waves can be produced in bounded domains and pattern formation varying in time can also be generated. This section is devoted to the analysis of some particular cases in R^1. The solutions obtained with the classical equations will be compared with the solutions with the bi-flux hypothesis.

The classical Gray-Scott model (Pearson, 1993; Lee *et al.* 1994) reads:

$$\frac{\partial q(x,t)}{\partial t} = \frac{\partial^2 q(x,t)}{\partial x^2} - qv^2 + A(1-q) \tag{7.3a}$$

$$\frac{\partial v(x,t)}{\partial t} = \delta^2 \frac{\partial^2 v(x,t)}{\partial x^2} + qv^2 - Bv \tag{7.3b}$$

The values of the parameters are given as: $\delta^2 = 0.01$, $A = 0.01$, $B = 0.053$. Consider the problem with the initial distribution given by:

$$q(x,0) = 1 - 0.5\sin^{100}(\pi x/100) \tag{7.4a}$$

$$v(x,0) = 0.25\sin^{100}(\pi x/100) \tag{7.4b}$$

as shown in Fig. 7.3

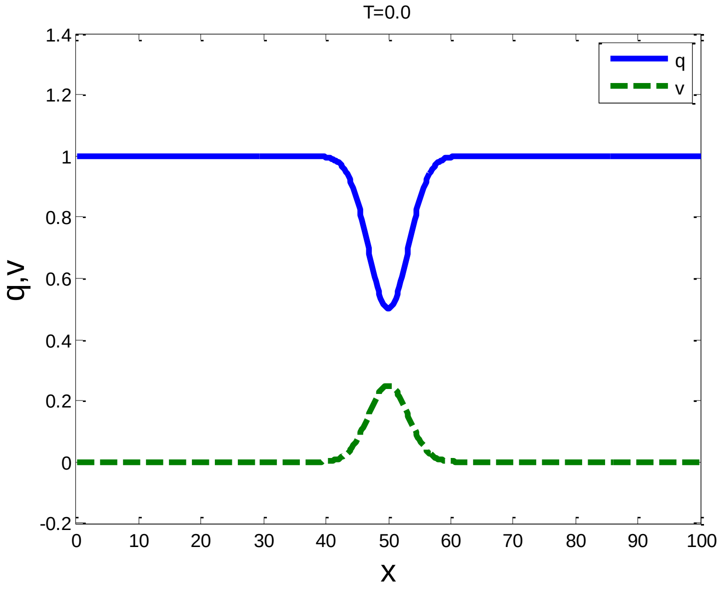


Fig.7.3 The initial distribution for the Gray-Scott model

The boundary conditions are given by no flux at x=0 and x=100 for both variables. That is:

$$\left.\frac{\partial q}{\partial x}\right|_{x=0} = \left.\frac{\partial v}{\partial x}\right|_{x=0} = 0 \qquad \text{and} \qquad \left.\frac{\partial q}{\partial x}\right|_{x=100} = \left.\frac{\partial v}{\partial x}\right|_{x=100} = 0$$

The nonlinear Galerkin method is used to obtain the numerical solution. The results for some selected time values are given in Fig.7.4. Comparison with the solution presented in (Doelman, 1997; Zhang, 2016) show that the results are very much similar.

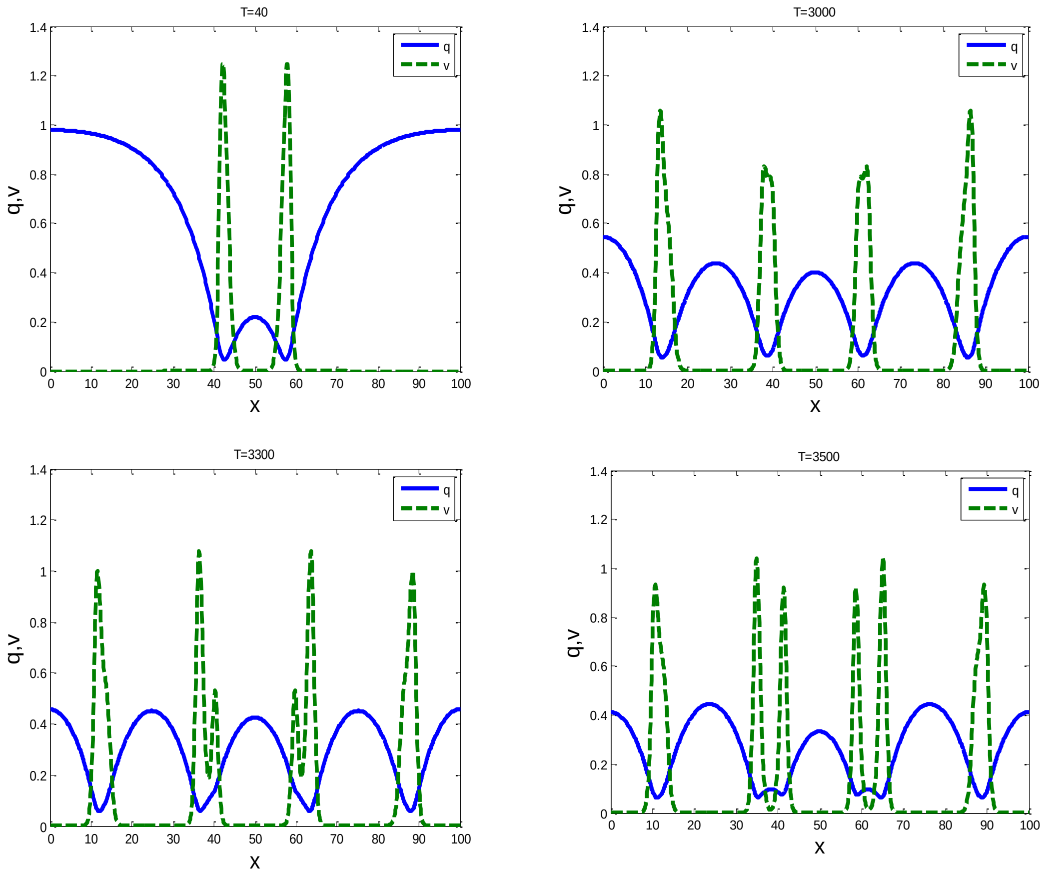


Fig.7.4 The evolution of q and v for the classical case

Now, we will consider the Gray-Scott model considering the bi-flux hypothesis which includes the fourth order in both equations. The new system reads:

$$\frac{\partial q(x,t)}{\partial t} = \beta_q D_q \frac{\partial^2 q(x,t)}{\partial x^2} - \beta_q (1-\beta_q) R_q \frac{\partial^4 q(x,t)}{\partial x^4} - qv^2 + A(1-q) \tag{7.5a}$$

$$\frac{\partial v(x,t)}{\partial t} = \delta^2 \beta_v \frac{\partial^2 v(x,t)}{\partial x^2} - \beta_v (1-\beta_v) R_v \frac{\partial^4 v(x,t)}{\partial x^4} + qv^2 - Bv \tag{7.5b}$$

Clearly as compared with the classical Gray-Scott model, the parameters β_q, β_v, R_q, R_v, D_q are added in this new model. In order to check the differences between these two models, the value of the parameters are imposed to be: $\delta^2 \beta_v = 0.01$,$\beta_q D_q = 1.0$, $A = 0.01, B = 0.053$, $\beta_q (1-\beta_q) R_q = 0.01, \beta_v (1-\beta_v) R_v = 0.01$.

For sake of simplicity, the value of β_q, β_v are put equal to 0.5. The other parameters are defined as: $\delta^2 = 0.02$, $D_q = 2$, $R_q = 0.04$, $R_v = 0.04$.

The initial conditions are the same as before and the boundary conditions are extended to include the non-flux condition to the secondary flux:

$$\left.\frac{\partial^3 q}{\partial x^3}\right|_{x=0} = \left.\frac{\partial^3 v}{\partial x^3}\right|_{x=0} = 0 \quad \text{and} \quad \left.\frac{\partial^3 q}{\partial x^3}\right|_{x=100} = \left.\frac{\partial^3 v}{\partial x^3}\right|_{x=100} = 0$$

As in the previous cases the fourth order partial differential equations (7.5) are transformed into a four second order equations system:

$$\frac{\partial^2 q(x,t)}{\partial x^2} = s \tag{7.6a}$$

$$\frac{\partial q(x,t)}{\partial t} = \beta_q D_q \frac{\partial^2 q(x,t)}{\partial x^2} - \beta_q (1-\beta_q) R_q \frac{\partial^2 s(x,t)}{\partial x^2} - qv^2 + A(1-q) \tag{7.6b}$$

$$\frac{\partial^2 v(x,t)}{\partial x^2} = u \tag{7.6c}$$

$$\frac{\partial v(x,t)}{\partial t} = \delta^2 \beta_v \frac{\partial^2 v(x,t)}{\partial x^2} - \beta_v (1-\beta_v) R_v \frac{\partial^2 u(x,t)}{\partial x^2} + qv^2 - Bv \tag{7.6d}$$

Note that

$$\left.\frac{\partial s}{\partial x}\right|_{x=0} = \left.\frac{\partial u}{\partial x}\right|_{x=0} = 0 \quad \text{and} \quad \left.\frac{\partial s}{\partial x}\right|_{x=100} = \left.\frac{\partial u}{\partial x}\right|_{x=100} = 0$$

The initial conditions $\left.\partial^2 q/\partial x^2\right|_{t=0} = \partial^2 q(x,0)/\partial x^2$ and $\left.\partial^2 v/\partial x^2\right|_{t=0} = \partial^2 v(x,0)/\partial x^2$ are obtained from the equations (7.4a,b)

The solutions of the system (7.6a,b,c,d) for t=40 and t=140 are given in the Fig.7.5.

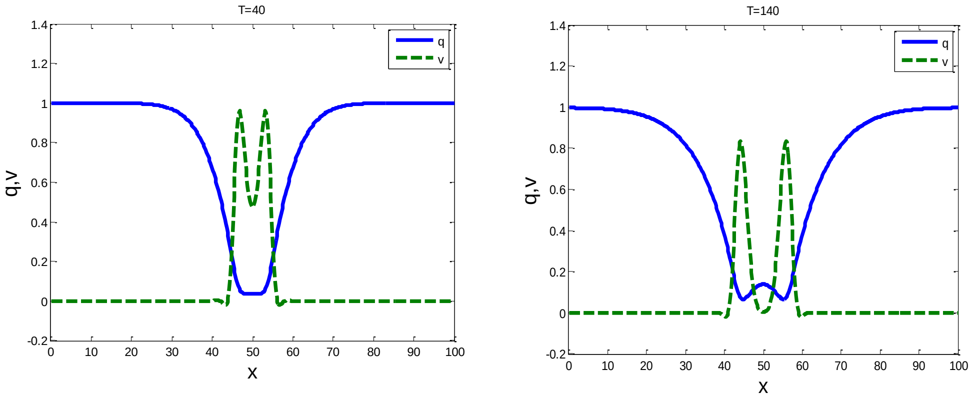


Fig.7.5 The evolution of q and v in the system at time T=40 and T=140

Comparing with the classical Gray-Scott solution, Fig.7.4, we can see that at time t=40, the bi-flux Gray-Scott model introduces a delay in the process of the variety self-replicating patterns ν. On the other rand the evolution of the variety q progresses in the opposite direction and is raised as compared with the classical solution.

It is also remarkable the regularity of the solution imposed by the bi-flux approach. For t=3000 and t=4500. The bi-flux solution imposes a very regular pattern on the pulses for both the self-replicating variable ν and the variable q as shown in the Fig.7.6. The classical solution introduces two more pulses for ν and destroys the symmetry of this variable. The variable q is also perturbed although less intensively then ν.

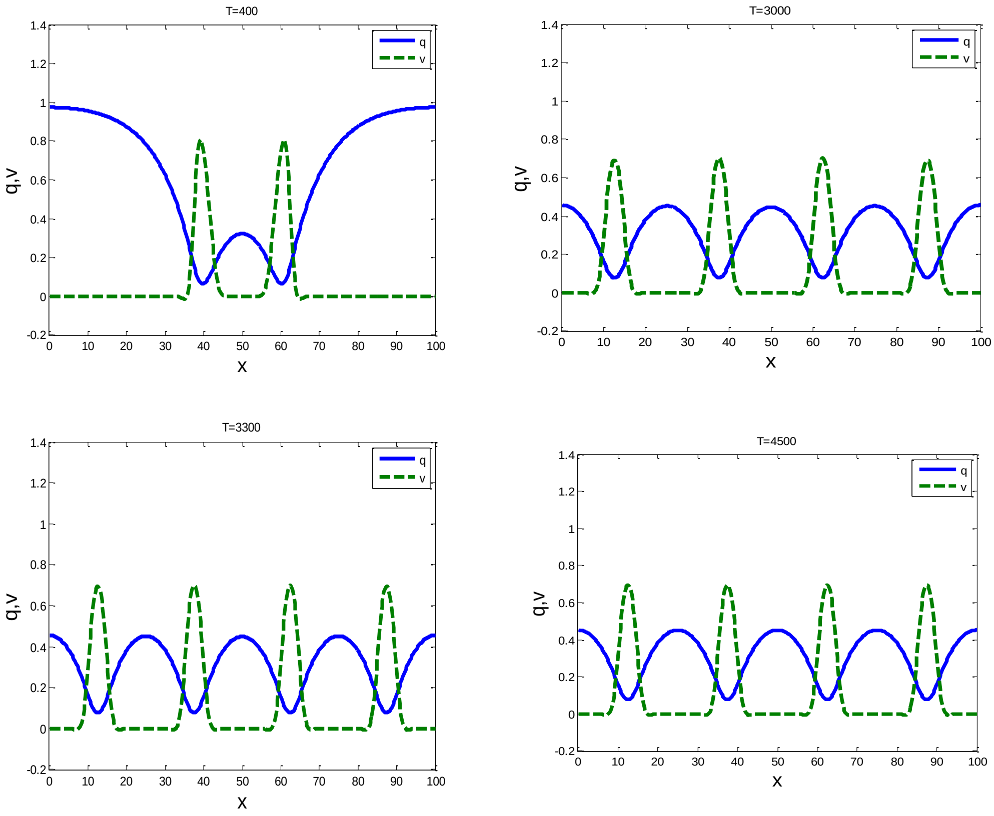


Fig.7.6 The evolution of q and v in the system at time T=400, 3000, 3300, 4500

As usual, the bi-flux approach introduces the anomaly related to negative values of the distribution, in this case referring to the self-replicating variable. Therefore for physically consistent solutions the initial condition related to ν must be sustained by a thin layer distributed on the domain of definition.

Assuming a new set of parameters given by: $\delta^2\beta_v = 0.01, \beta_q D_q = 1.0$, $A = 0.02$, $B = 0.04$, $\beta_q(1-\beta_q)R_q = 1.1, \beta_v(1-\beta_v)R_v = 0.05$, the numerical solution is qualitatively similar but with a larger number of pulses as shown in the Fig. 7.7 and

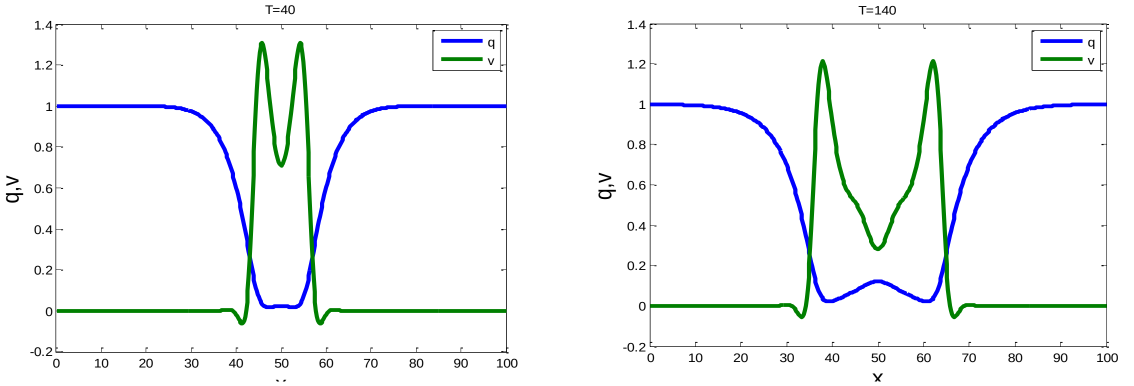


Fig.7.7 The evolution of q and v in the system at time T=40,140

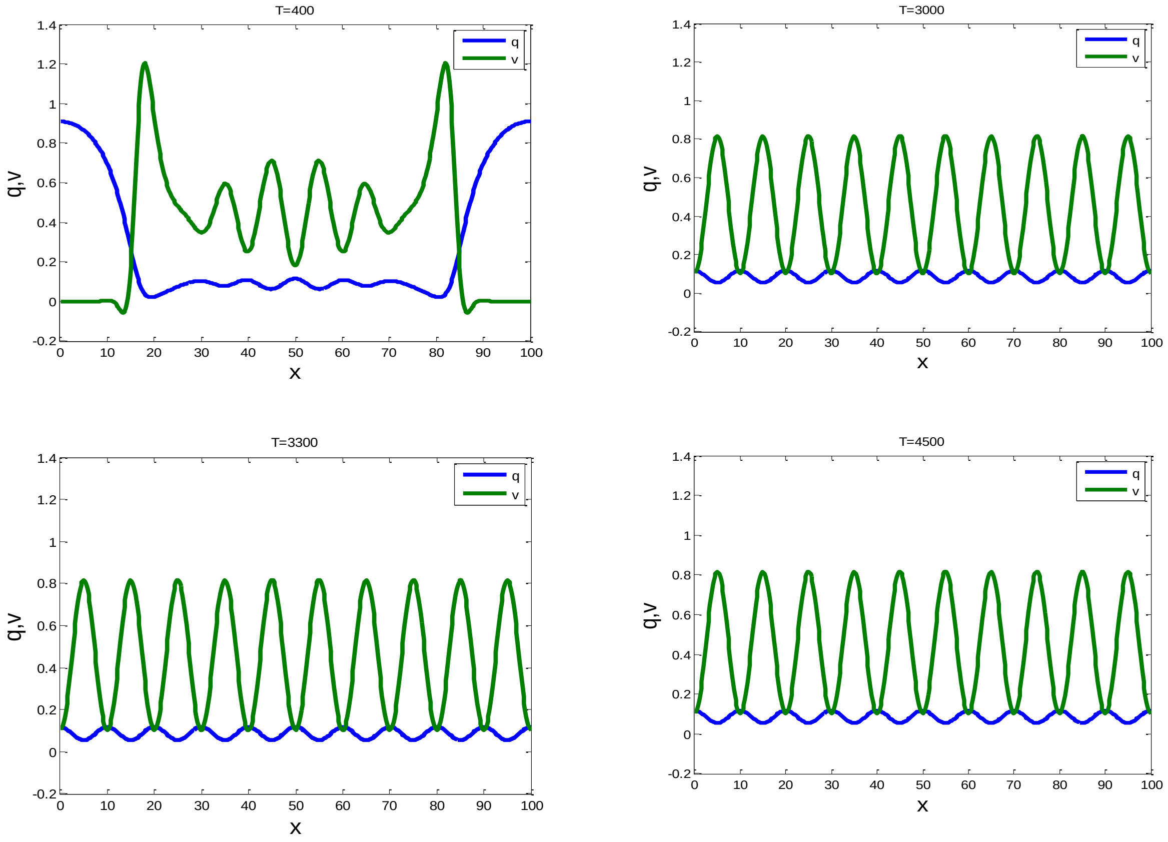


Fig.7.8 The evolution of q and v in the system at time T=400, 3000, 3300, 4500

7.8.

As in the previous examples convergence tests were used to evaluate the performance of the numerical method. Consider the system:

$$\frac{\partial q(x,t)}{\partial t} = \beta_q D_q \frac{\partial^2 q(x,t)}{\partial x^2} - \beta_q\left(1-\beta_q\right)R_q \frac{\partial^4 q(x,t)}{\partial x^4} - qv^2 + A(1-q) + f_{11}(q,v)$$

$$\frac{\partial v(x,t)}{\partial t} = \delta^2 \beta_v \frac{\partial^2 v(x,t)}{\partial x^2} - \beta_v(1-\beta_v)R_v \frac{\partial^4 v(x,t)}{\partial x^4} + qv^2 - Bv + g_{11}(q,v)$$

Where

$$\begin{aligned} f_{11}(q,v) = {} & \left(\beta_q D_q \pi^2 + \beta_q\left(1-\beta_q\right)R_q \pi^4 - 1\right)\cos(\pi x)\exp(-t) + \cos(\pi x)\cos(2\pi x)\exp(-3t) \\ & + A\left(1-\cos(\pi x)\exp(-t)\right) \end{aligned}$$

$$\begin{aligned} g_{11}(q,v) = {} & \left(\delta^2 \beta_v \pi^2 + \beta_v\left(1-\beta_v\right)R_v \pi^4 - 1\right)\cos(2\pi x)\exp(-t) - \cos(\pi x)\cos(2\pi x)\exp(-3t) \\ & + B\cos(2\pi x)\exp(-t) \end{aligned}$$

The initial condition given as $q(x,0) = \cos(\pi x); v(x,0) = \cos(2\pi x)$, with no flux boundary condition. The analytical solution can be found:

$$q(x,t) = \cos(\pi x)\exp(-t);$$

$$v(x,t) = \cos(2\pi x)\exp(-t)$$

Now, take $\partial^2 q(x,t)/\partial x^2 = s(x,t), \partial^2 v(x,t)/\partial x^2 = u(x,t)$ to define the system into four second order equations:

$$\frac{\partial^2 q(x,t)}{\partial x^2} = s(x,t)$$

$$\frac{\partial q(x,t)}{\partial t} = \beta_q D_q \frac{\partial^2 q(x,t)}{\partial x^2} - \beta_q\left(1-\beta_q\right)R_q \frac{\partial^2 s(x,t)}{\partial x^2} - qv^2 + A(1-q) + f_{11}(q,v)$$

$$\frac{\partial^2 v(x,t)}{\partial x^2} = u(x,t)$$

$$\frac{\partial v(x,t)}{\partial t} = \delta^2 \beta_v \frac{\partial^2 v(x,t)}{\partial x^2} - \beta_v(1-\beta_v)R_v \frac{\partial^2 u(x,t)}{\partial x^2} + qv^2 - Bv + g_{11}(q,v)$$

The value of the constants given by $\delta^2 \beta_v = 0.01$ $, \beta_q D_q = 1.0$, $A = 0.01, B = 0.053$, $\beta_q\left(1-\beta_q\right)R_q = 0.01, \beta_v(1-\beta_v)R_v = 0.01$.

Table 7.2a CPU time, error and order of accuracy for q in Gray-Scott model with bi-flux under nonlinear Galerkin method

N	h	Δt	CPU(s)	L_∞ for q	Order	L_2 for q	Order
5	0.2	0.04	0.059	1.47e-002		1.15e-002	
10	0.1	0.01	0.192	3.67e-003	2.00	2.60e-003	2.15
20	0.05	0.0025	1.219	9.12e-004	2.01	6.19e-004	2.07
40	0.025	6.25e(-4)	9.0247	2.27e-004	2.01	1.51e-004	2.04
80	0.0125	1.56e(-4)	71.891	5.67e-005	2.00	3.72e-005	2.02
160	0.0063	3.91e(-5)	572.98	1.42e-005	2.00	9.25e-006	2.01

Table 7.2b CPU time, error and order of accuracy for v in Gray-Scott model with bi-flux under nonlinear Galerkin method

N	h	Δt	CPU(s)	L_∞ for v	Order	L_2 for v	Order
5	0.2	0.04	0.059	4.48e-002		3.03e-002	
10	0.1	0.01	0.192	1.21e-002	1.89	7.55e-003	2.01
20	0.05	0.0025	1.219	3.08e-003	1.97	1.83e-003	2.05
40	0.025	6.25e(-4)	9.0247	7.72e-004	2.00	4.49e-004	2.03
80	0.0125	1.56e(-4)	71.891	1.93e-004	2.00	1.11e-004	2.02
160	0.0063	3.91e(-5)	572.98	4.83e-005	2.00	2.76e-005	2.01

From the table 7.2a,b and Fig.7.8a,b, we can find that the convergence order of this method is two. Also, these results represent good accuracy and confirm the robustness of the method. The error decreases exponentially with increasing number of elements.

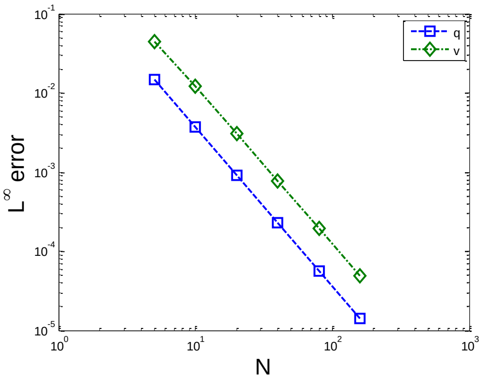


Fig.7.9a Cell N vs L_∞ error

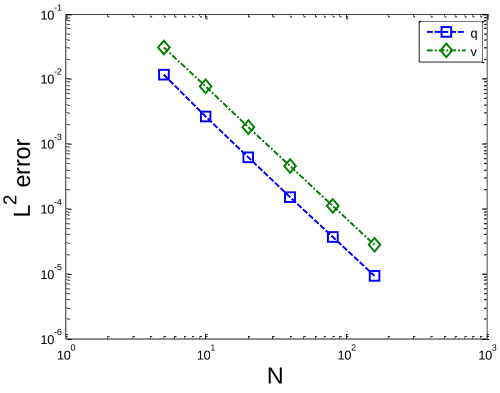


Fig.7.9b Cell N vs L_2 error

In this chapter it was shown the influence of the fourth order equation modeling the bi-flux phenomenon for two cases of non-linear equations. The non-linearity for both cases was concerned to the source/sink terms. Other non-linear cases particularly concerning the interaction between the reactivity coefficient R and the concentration q(x,t) deserve to be analyzed. These cases however fall beyond the scope of the present work.

Our purpose was to show that the bi-flux theory interferes in the solution preserving the fundamental behavior of the classical case for some important situations.

Chapter 8

Conclusions and Future Work

The discrete process of diffusion with retention in a two dimensional domain was developed to obtain the fourth order equation, which suggests the introduction of a secondary flux leading to a bi-flux theory. The secondary flux was introduced in the mass conservation principle to obtain a fourth order equation as shown in Chapter 2. As suggested in Chapters 3 and 4, the dependence of R and β is critical both for isotropic and anisotropic media. For isotropic media the delay or acceleration of diffusion processes depends strongly from the relation R-β. For anisotropic media the relation $\beta=\beta(R)$ is still more important. It was clearly shown that, at least for closed domains, no flux at the boundaries, the reactivity coefficient plays the role of an attractor provided that β is a decreasing function of R

The anomaly of the distribution developing negative values for the concentration after the introduction of initial conditions highly concentrated at a given point far from the boundaries is recurrent for one- and two-dimensional cases. It was shown however that there is a critical initial concentration $q_{crit}(x,0)$ separating the behavior into $q(x,t)>0$ for all x and $q(x^*,t)<0$ for some interval $[x_e<x^*<x_d]$. Two selected examples were introduced. The first is related to the initial condition $q(x,0)=[0.5(1+\cos(\pi x))]^n$, subject to the no flux boundary condition; the second is related to the initial condition $q(x,0)=[\cos(0.5\pi x)]^n$. The boundary conditions impose the concentration q and its second derivative to vanish at the boundaries. For n less than some critical value the solution is regular. Therefore there must a critical n such that for $n< n_{crit}$ the solution is regular. This result may be a starting point for a mathematical analysis intended to explain the necessary conditions for developing negative values.

An extremely important conclusion is the criticality of the definition of secondary flux. It was shown that there are three classes of definition. For the first class the influence on the concentration evolution is not critical. But for the second and third classes the influence on the time variation of the concentration for certain initial conditions in anisotropic media $R=R(x,y)$ is critical. The second and third class definition for the secondary flux leads to an unexpected increasing in the concentration in regions with negative distribution gradients which is impossible for the classical approach. The difference in the behaviors induced by the definitions of the secondary flux is due to the perturbation on the first and second derivatives of $q(x,t)$ arising from the variation of R and β as functions of x. These terms combine with the terms coming from the primary flux coefficients. There is therefore a spurious influence of the parameters corresponding to the secondary flux into the primary flux. The definition that seems to be appropriate for the secondary flux is to consider the respective flux potential proportional to curvature that is proportional to ($\beta\Delta q$). With this definition $\boldsymbol{\Psi}_2=R\{[(\partial(\beta\Delta q)/\partial x]\boldsymbol{i}+[(\partial(\beta\Delta q)/\partial y]\boldsymbol{j}\}$.

After several solutions for non-flux boundary conditions it becomes clear that the the reactivity coefficient $R(x)$ for anisotropic media plays the role of an attractor. Clearly the partition β is a decreasing function of R. This property suggests that the reactivity in problems related to population dynamics can considered as a nutrient box attracting biological particles. In this sense it was also propose a model that considers the reactivity coefficient varying in space and time according to a diffusion process.

This new approach admits the existence of two simultaneous fluxes. It is not two distinct sets of particles scattering with different velocities but particles with the same general physical characteristics diffusing in two distinct energy states E_1 and E_2. The particles may transfer from one state to the other depending on some intrinsic physic-chemical property or due to the action of external fields. Two new physical constants are introduced namely, the reactivity coefficient R and the parameter β representing the partition of the flux in two groups. That is a fraction β of particles scatters in the state E_1 and the complementary fraction ($1-\beta$) scatters in the energy state E_2. In chapter 6, it is presented a brief discussion about an ideal evolution of energy states associated to the exchange of kinetic energy. It is assumed that translational energy and rotational energy could exchange with each other. Considering an ideal universe the idea of a particular type of entropy is proposed which is consistent with the usual definition of entropy in thermodynamics. The basic concepts and dynamics of diffusion considering rotational energy has however to be further explored. A few publications (Bevilacqua *et al.*, 2016) deal with this topic which is rather complex. It is necessary to put much more effort to advance this type of behavior. Probably the bi-flux approach could contribute to advance the theory of diffusion of particles with rotation.

For some non-linear processes the bi-flux approach as an extension of the classical postulation preserves the dominant characteristics of the classical solution introducing interesting regularization as in the Gray-Scott problem.

As suggestion for future work it is to be highlighted:

1. Try to institute an appropriated master equation with inclusion of random variables. It should be possible to make use of some basic principles of the mathematical physics.
2. The relation between R and β should be further analyzed. It seems that it is very difficult to establish general laws for the interdependence of these two parameters. The relation $\beta=\beta(R)$ should be representative of each context, socio-economic, biological, physico-chemical.

3. The property of $R(x)$ for anisotropic media as an attractor should be further analyzed. Some analytical justification should be searched.
4. The anomalies corresponding to negative values of the concentration should be further investigated with the help of the numerical results.
5. The steady state solutions should be determined. It is much more complex than the steady state for the classical case. Of particular interest is the term $R\beta(1-\beta)$ which is the logistic equation that could induce chaotic behavior.
6. The extension of the problem with the inclusion of the dependence of the new parameters on the concentration is also of great interest. It is possible for the reactivity coefficient to be strongly dependent on $q(x,t)$
7. Another important point that is missing, and is critical for the discussion in a broader academic context, is the search for applications. I think that biological processes and medical applications like the evolution of tumors are appropriated topics to be explored with this theory. Also flux of capital seems to be an attractive topic to be dealt with this theory.

Finally I would say that most of all it is necessary to establish a network of researchers and students interested in problems related to diffusion. They should come from different fields of interest. I think that this theme is extremely rich and can turn to be an important source for research lines.

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Appendix

A Numerical scheme for linear equation

A1. The Galerkin finite element method with Hermite element

In this part, we will consider how to use finite element method to get the numerical solution. Consider the equation as below, $\mathbf{x} \in R^2$:

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = \nabla(\beta D \nabla q(\mathbf{x},t)) - \nabla(\beta(1-\beta)R\nabla(\Delta q(\mathbf{x},t))) \qquad \text{(A-1a)}$$

$$q(\mathbf{x},0) = q_0(\mathbf{x}),\ \mathbf{x} \in \Omega; \qquad \text{(A-1b)}$$

$$\nabla q(\mathbf{x},t) = 0, \nabla^3 q(\mathbf{x},t) = 0,\ \mathbf{x} \in \partial\Omega \qquad \text{(A-1c)}$$

First, let $\Delta q(\mathbf{x},t) = p(\mathbf{x},t)$ and introduce into Eq.(A-1a,1c), we get:

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = \nabla(\beta D \nabla q(\mathbf{x},t)) - \nabla(\beta(1-\beta)R\nabla(p(\mathbf{x},t))) \qquad \text{(A-2a)}$$

$$\Delta q(\mathbf{x},t) = p(\mathbf{x},t) \qquad \text{(A-2b)}$$

$$q(\mathbf{x},0) = q_0(\mathbf{x}),\ \mathbf{x} \in \Omega; \qquad \text{(A-2c)}$$

$$\nabla q(\mathbf{x},t) = 0, \nabla p(\mathbf{x},t) = 0,\ \mathbf{x} \in \partial\Omega \qquad \text{(A-2d)}$$

With the weighted integral statement for the Eq. (A-2a, 2b, 2c), we can get:

$$\int_\Omega \frac{\partial q(\mathbf{x},t)}{\partial t} \omega d\mathbf{x} = \int_\Omega (\nabla(\beta D \nabla q(\mathbf{x},t)) - \nabla(\beta(1-\beta)R\nabla(p(\mathbf{x},t))))\omega d\mathbf{x}$$

$$\int_{\Omega} \Delta q(\mathbf{x},t)\omega d\mathbf{x} = \int_{\Omega} p(\mathbf{x},t)\omega d\mathbf{x}$$

Where, $\omega \in H^1(\Omega)$. $H^1(\Omega)$ is the Hilbert space. Then the above system is simplified by Green theory to give:

$$\begin{aligned} \int_{\Omega} \frac{\partial q(\mathbf{x},t)}{\partial t}\omega d\mathbf{x} &= \int_{\partial\Omega} \beta D \nabla q(\mathbf{x},t)\omega d\mathbf{x} - \int_{\Omega} \beta D \nabla q(\mathbf{x},t)\nabla\omega d\mathbf{x} - \\ &\int_{\partial\Omega} \beta(1-\beta)R\nabla p(\mathbf{x},t)\omega d\mathbf{x} + \int_{\Omega} \beta(1-\beta)R\nabla p(\mathbf{x},t)\nabla\omega d\mathbf{x} \end{aligned} \tag{A-3a}$$

$$\int_{\Omega} \nabla q(\mathbf{x},t)\nabla\omega d\mathbf{x} + \int_{\Omega} p(\mathbf{x},t)\omega d\mathbf{x} - \int_{\partial\Omega} \nabla q(\mathbf{x},t)\omega d\mathbf{x} = 0 \tag{A-3b}$$

Subject to the boundary condition, the system above can be rewritten as:

$$\int_{\Omega} \frac{\partial q(\mathbf{x},t)}{\partial t}\omega d\mathbf{x} = -\int_{\Omega} \beta D \nabla q(\mathbf{x},t)\nabla\omega d\mathbf{x} + \int_{\Omega} \beta(1-\beta)R\nabla p(\mathbf{x},t)\nabla\omega d\mathbf{x} \tag{A-4a}$$

$$\int_{\Omega} \nabla q(\mathbf{x},t)\nabla\omega d\mathbf{x} + \int_{\Omega} p(\mathbf{x},t)\omega d\mathbf{x} = 0 \tag{A-4b}$$

A2 Solution with Hermite finite element for one dimensional case under D, R and β constants.

For 1D domain, the cubic Hermite base functions for the reference element $I_0 = [-1,1]$ are given as:

$$H_1 = \frac{1}{4}\left(2 - 3\xi + \xi^3\right)$$

$$H_1(-1) = 1,\ H_1(1) = H_1(-1) = H_1(1) = 0$$

$$H_2 = \frac{1}{4}\left(1 - \xi - \xi^2 + \xi^3\right)$$

$$H_2'(-1) = 1,\ H_2(1) = H_2(-1) = H_2'(1) = 0$$

$$H_3 = \frac{1}{4}\left(2 + 3\xi - \xi^3\right)$$

$$H_3(1) = 1,\ H_3(-1) = H_3'(-1) = H_3'(1) = 0$$

$$H_4 = \frac{1}{4}\left(-1 - \xi + \xi^2 + \xi^3\right)$$

$$H_4'(1) = 1,\ H_4(1) = H_4(-1) = H_4'(1) = 0$$

Where $H_i'(\xi_0), i = 1,2,3,4$ means the value of the first derivative at the point ξ_0. We denote the unknowns by $q_1^j, q_2^j; p_1^j, p_2^j$ to represent the values of $q, q_x; p, p_x$ at the point j , $j = 1,2$. Then the approximated solution $q_h(x)$ and $p_h(x)$ for the Galerkin method inside the reference domain can be expressed respectively as :

$$q_h(\xi) = \sum_{j=1}^{2} q_1^j H_j(\xi) + q_2^j(\xi) H_{j+2}$$

$$p_h(\xi) = \sum_{j=1}^{2} p_1^j H_j(\xi) + p_2^j(\xi) H_{j+2}$$

$$\omega_i = H_i \,.\, i = 1,2,3,4$$

The finite element approximation for (A-4) can be expressed as:

$$M\dot{Q} = \beta D \cdot KQ + \beta(1-\beta) R \cdot KP \tag{A-5a}$$

$$KQ + MP = 0 \tag{A-5b}$$

Where, $\dot{Q}$ means the partial derivative with respect to time. M and K are the mass matrix and stiffness matrix in the original domain, respectively. Let $(\cdot,\cdot)$ denote the usual scalar L^2 inner product. Given as:

$$\left(H_i, H_j\right) = \int_{-1}^{1} H_i \cdot H_j dx$$

$$\left(\nabla H_i, \nabla H_j\right) = \int_{-1}^{1} \frac{\partial H_i}{\partial x} \cdot \frac{\partial H_j}{\partial x} dx, \quad i = 1,2\,,\ j = 1,2$$

Because each computational grid on the reference domain has 4 degrees of the freedom, this leads to a system of 4×4 coupling equations. Thus 4×4block mass matrix m and stiffness matrix k in the reference domain are defined as follows:

$$m = \begin{pmatrix} (H_1, H_1) & (H_1, H_2) \\ (H_2, H_1) & (H_2, H_2) \end{pmatrix}$$

$$k = \begin{pmatrix} (\nabla H_1, \nabla H_1) & (\nabla H_1, \nabla H_2) \\ (\nabla H_2, \nabla H_1) & (\nabla H_2, \nabla H_2) \end{pmatrix}$$

Considered the computational sub-interval $I = \lfloor x_i, x_j \rfloor$, the calculation of the integration in $I = \lfloor x_i, x_j \rfloor$ is performed reducing the operation to the reference interval I_0.

The affine relation between I and I_0 can be chosen as :

$$x = \frac{x_j - x_i}{2}\xi + \frac{x_j + x_i}{2}$$

Thus, $dx = \frac{x_j - x_i}{2} d\xi$, $J = \frac{d\xi}{dx} = \frac{x_j - x_i}{2}$.

The integral on the domain could be written as the sum on all sub-intervals for equation (A-4). In general the integration on each subinterval will be performed after transforming the actual coordinates into the corresponding ones in the reference domain I$_0$. The integration can then be easily evaluated with four point Gaussian quadrature rule on I_0:

$$\int_I q_h(x,t)\omega dx = \int_{x_i}^{x_j} q_h(x,t)\omega dx = \int_{-1}^{1} q_h(\xi,t)\omega |J| d\xi$$

$$\int_I \nabla q_h(x,t) \nabla \omega dx = \int_{x_i}^{x_j} \nabla q_h(x,t) \nabla \omega dx = \int_{-1}^{1} \nabla q_h(\xi,t) \nabla \omega |J| d\xi$$

Where $|J| = \left|\frac{d\xi}{dx}\right| = \frac{x_j - x_i}{2}$ is a Jacobian determinant. The discrete solution vectors Q, P are defined as:

$$Q = \left[q^1, q_x^1, \cdots, q^{n+1}, q_x^{n+1}\right], P = \left[p^1, p_x^1, \cdots, p^{n+1}, p_x^{n+1}\right].$$

The matrices M and K, which are the global mass matrix and the global stiffness matrix, depend on the local mass and stiffness matrices m and k, respectively. The relationship is defined by the number of points linking the global number in the original domain and the local number in the subdomain. Until this point, the equations (A-5a) and (A-5b) comprise a system of time dependent ordinary differential equations. This system can be solved with several numerical methods, like as Euler's methods, Runge-Kutta method, Newmark-beta method etc. Here, we will use the simple Euler backward difference algorithm. The full discrete formulation can be written as:

$$MQ^{t+1} - MQ^t = \Delta t\left(-\beta D \cdot KQ^{t+1} + \beta(1-\beta)R \cdot KP^{t+1}\right) \qquad \text{(A-6a)}$$

$$KQ^{t+1} + MP^{t+1} = 0 \qquad \text{(A-6b)}$$

Then, can be rewritten in martrix form as:

$$\begin{bmatrix} M + \Delta t\beta D \cdot K & -\Delta t\beta(1-\beta)R \cdot K \\ K & M \end{bmatrix}\begin{bmatrix} Q \\ P \end{bmatrix}^{t+1} = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} Q \\ P \end{bmatrix}^{t} \qquad \text{(A-7)}$$

The initial distribution Q^0 and P^0 are obtained from the conditions determined by (A-2c) and (A-2b), respectively. Then numerical solution of this system is performed with the platform Matlab.

A3 The coefficients are constant for two dimensional case with BFS element

In 2D case, for the spatial domain, the Bogner-Fox-Schmidt (BFS) element will be employed because it leads directely to the determination of the concentration and the primary and secondary fluxes as in one dimensional case. It is used the Lagrange element with the advantage of less computational time. The process for assembling the algorithm is similar to that used for the one dimension case. The base functions called cubic Hermite function of Bogner-Fox-Schmidt (BFS) element are write for the reference element on $[-1,1]\times[-1,1]$, subject to the point $(\xi,\eta)\in[-1,1]\times[-1,1]$.

$$BS_{11}=H_1(\xi)H_1(\eta)\ ,\ BS_{21}=H_3(\xi)H_1(\eta),\ BS_{31}=H_3(\xi)H_3(\eta), BS_{41}=H_1(\xi)H_3(\eta)$$

$$BS_{12}=H_2(\xi)H_1(\eta),\ BS_{22}=H_4(\xi)H_1(\eta), BS_{32}=H_4(\xi)H_3(\eta), BS_{42}=H_2(\xi)H_3(\eta)$$

$$BS_{13}=H_1(\xi)H_2(\eta),\ BS_{23}=H_3(\xi)H_2(\eta), BS_{33}=H_3(\xi)H_4(\eta), BS_{43}=H_1(\xi)H_4(\eta)$$

$$BS_{14}=H_2(\xi)H_2(\eta),\ BS_{24}=H_4(\xi)H_2(\eta), BS_{34}=H_4(\xi)H_4(\eta), BS_{44}=H_2(\xi)H_4(\eta)$$

Where, the value of ξ belongs to $[-1,1]$, and the the value of η as well.

$H_1(\xi)=\frac{1}{4}\left(2-3\xi+\xi^3\right)$, $H_2(\xi)=\frac{1}{4}\left(1-\xi-\xi^2+\xi^3\right)$, $H_3(\xi)=\frac{1}{4}\left(2+3\xi-\xi^3\right)$ $H_4(\xi)=\frac{1}{4}\left(-1-\xi+\xi^2+\xi^3\right)$ are the base Hermite polynomial in one dimensional case.

For the base functions in the square domain, the process is similar to that used in the one dimension case. For instance, the four base functions BS_{11}, BS_{12}, BS_{13}, BS_{14} subject to the restrictions for the point $(-1,-1)$, that is $\xi=-1$ and $\eta=-1$ should match the conditions:

$$BS_{11}(-1,-1)=1,\ BS_{11\xi}(-1,-1)=BS_{11\eta}(-1,-1)=BS_{11\xi\eta}(-1,-1)=0$$

$$BS_{12\xi}(-1,-1)=1,\ BS_{12}(-1,-1)=BS_{12\eta}(-1,-1)=BS_{12\xi\eta}(-1,-1)=0$$

$$BS_{13\eta}(-1,-1)=1,\ BS_{13}(-1,-1)=BS_{13\xi}(-1,-1)=BS_{13\xi\eta}(-1,-1)=0$$

$$BS_{14\xi\eta}(-1,-1)=1,\ BS_{14}(-1,-1)=BS_{14\xi}(-1,-1)=BS_{14\eta}(-1,-1)=0$$

Where $BS_{11\xi}$ denotes the first partial differential of $BS_{11}(\xi,\eta)$ with respct to the ξ coordinate; $BS_{11\eta}$ denotes the first partial differential for $BS_{11}(\xi,\eta)$ with respct to the η

coordinate; $BS_{11\xi\eta}$ denotes the second mixed partial differential of $BS_{11}(\xi,\eta)$ with respct to the ξ and η coordinates.

The other base functions BS_{21}, BS_{22}, BS_{23}, BS_{24}; BS_{31}, BS_{32}, BS_{33}, BS_{34}; BS_{41}, BS_{42}, BS_{43}, BS_{44} referring to the points $(1,-1);(-1,1);(1,1)$ respectively are determined following similar reazoning as before referring to point $(-1,-1)$

For the uniform mesh sizes $h_x = x_i - x_{i-1}$ in the x direction and $h_y = y_i - y_{i-1}$ in the y direction, we introduce the unknowns $q_1^j, q_2^j, q_3^j, q_4^j$ to represent the value of q, q_x, p_y, p_x at the point j, $j = 1,2,3,4$, respectively. So that the approximate solution $q_h(x,y)$ and $p_h(x,y)$ for the Galerkin method inside the reference domain can be expressed as :

$$q_h(\xi,\eta) = \sum_{j=1}^{4} BS_{j1} q_1^j + BS_{j2} q_2^j h_x + BS_{j3} q_3^j h_y + BS_{j4} q_4^j h_x h_y$$

$$p_h(\xi,\eta) = \sum_{j=1}^{4} BS_{j1} p_1^j + BS_{j2} p_2^j h_x + BS_{j3} p_3^j h_y + BS_{j4} p_4^j h_x h_y$$

For the two dimensional case, $(\cdot,\cdot)$ the usual scalar L^2 inner product is given as:

$$(BS_{ij}, BS_{st}) = \int_{-1}^{1}\int_{-1}^{1} BS_{ij} \cdot BS_{st} d\xi d\eta$$

$$(\nabla BS_{ij}, \nabla BS_{ij}) = \int_{-1}^{1}\int_{-1}^{1} \frac{\partial BS_{ij}}{\partial \xi} \cdot \frac{\partial BS_{st}}{\partial \xi} + \frac{\partial BS_{ij}}{\partial \eta} \frac{\partial BS_{st}}{\partial \eta} d\xi d\eta,$$

$$i = 1,\ldots,4,\ j = 1,\ldots,4,\ s = 1,\ldots,4,\ t = 1,\ldots,4$$

Since there is 16 degrees of freedom for the reference domain, the dimension of the mass matrix m and the stiffness martix k in is 16×16, respectively, and are given as:

$$m = \begin{pmatrix} (BS_{11}, BS_{11}) & \ldots & (BS_{11}, BS_{44}) \\ \vdots & (BS_{floor(i/4)+1, i \bmod 4}, BS_{floor(j/4)+1, j \bmod 4}) & \vdots \\ (BS_{41}, BS_{11}) & \ldots & (BS_{44}, BS_{44}) \end{pmatrix}$$

$$k = \begin{pmatrix} (\nabla BS_{11}, \nabla BS_{11}) & \ldots & (\nabla BS_{11}, \nabla BS_{44}) \\ \vdots & (\nabla BS_{floor(i/4)+1, i \bmod 4}, \nabla BS_{floor(j/4)+1, j \bmod 4}) & \vdots \\ (\nabla BS_{41}, \nabla BS_{11}) & \ldots & (\nabla BS_{44}, \nabla BS_{44}) \end{pmatrix}$$

$$i = 1,\ldots,16\,,\; j = 1,\ldots,16$$

Where “floor” for the subscript $i/4$ means the value of the nearest integer less than $i/4$ for instant, $floor(9/4) = 2$; $i \bmod 4$ means the remainder when i divided by 4, for instance, $13 \bmod 4 = 1$.

We assume that the computational sub-domain $\Omega^e = [x_{i-1}, x_i] \times [y_{i-1}, y_i]$ is affinely equivalent to the reference domain $\Omega^c = [-1,1] \times [-1,1]$. And the affine transformation is defined as:

$$T^e : \Omega^e \rightarrow \Omega^c$$

$$T^e(x, y) = \left(\frac{x - x_{i-1}}{h_x}, \frac{y - y_{i-1}}{h_y} \right) \equiv (\xi, \eta)$$

The numerical formulation used is same as in the one dimensional case, so that the integration in two dimensional space is written as:

$$\int_{\Omega^e} q_h(x,t)\omega dx = \int_{x_i}^{x_j} \int_{y_i}^{y_j} q_h(x,t)\omega dxdy = \int_{-1}^{1} \int_{-1}^{1} q_h(\xi,t)\omega |J| dxdy$$

$$\int_{\Omega^e} \nabla q_h(x,t) \nabla \omega dx = \int_{x_i}^{x_j} \int_{y_i}^{y_j} \nabla q_h(x,t) \nabla \omega dxdy = \int_{-1}^{1} \int_{-1}^{1} \nabla q_h(\xi,t) \nabla \omega |J| dxdy$$

Where $|J| = \begin{vmatrix} d\xi/dx & d\xi/dy \\ d\eta/dx & d\eta/dy \end{vmatrix}$ is a Jacobian determinant. The discrete solution vectors Q, P are defined as:

$$Q = \left[q^1, q_x^1, q_y^1, q_{xy}^1 \cdots, q^{n+1}, q_x^{n+1}, q_y^{n+1}, q_{xy}^{n+1}\right]\,,$$

$$P = \left[p^1, p_x^1, p_y^1, p_{xy}^1 \cdots, p^{n+1}, p_x^{n+1}, p_y^{n+1}, p_{xy}^{n+1}\right],$$

M and K are the mass matrix and stiff matrix in the original domain, respectively. For time integration, the Euler backward difference is used to estimate the solution for the semi-discrete equation (A-5), consequently, the full discrete model is obtained in matrix representation similarly as (A-7):

$$\begin{bmatrix} M + \Delta t \beta D \cdot K & -\Delta t \beta (1-\beta) R \cdot K \\ K & M \end{bmatrix} \begin{bmatrix} Q \\ P \end{bmatrix}^{t+1} = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q \\ P \end{bmatrix}^{t}$$

With the initial condition for the system (A-2c), the algorithm can be implemented starting with Q^0 and P^0 corresponding to $t = 0$ on the platform Matlab.

A4 Solution for constant coefficients for two dimensional case with Lagrange finite element

Comparing with A3, the difference is just the base function, here the Lagrange base function is employed on the reference domain for the spatial domain, the numerical method for time integration is the same that is the Euler's backward difference. Thus, the structure of the method is the same. We first list the base function on the reference domain $[-1,1]\times[-1,1]$, given as :

$$L_1(\xi,\eta)=\frac{1}{4}(1-\xi)(1-\eta),\ L_2(\xi,\eta)=\frac{1}{4}(1+\xi)(1-\eta)$$

$$L_3(\xi,\eta)=\frac{1}{4}(1+\xi)(1+\eta),\ L_4(\xi,\eta)=\frac{1}{4}(1-\xi)(1+\eta),$$

Then the approximated solution $q_h(x,y)$ and $p_h(x,y)$ for the Galerkin method inside the reference domain with Lagrange base function can be expressed as :

$$q_h(\xi,\eta)=\sum_{j=1}^{4} L_j q^j$$

$$p_h(\xi,\eta)=\sum_{j=1}^{4} L_j p^j$$

For the two dimensional case, $(\cdot,\cdot)$ the usual scalar L^2 inner product is given as:

$$(L_i, L_j)=\int_{-1}^{1}\int_{-1}^{1} L_i \cdot L_j d\xi d\eta$$

$$(\nabla L_i, \nabla L_j)=\int_{-1}^{1}\int_{-1}^{1} \frac{\partial L_i}{\partial \xi}\cdot\frac{\partial L_j}{\partial \xi}+\frac{\partial L_i}{\partial \eta}\frac{\partial L_j}{\partial \eta} d\xi d\eta,$$

$$i=1,\ldots,4,\ j=1,\ldots,4,$$

Since there are 4 degrees of freedom for the reference domain, the mass matrix m and stiff matrix k as in the one dimensional case are both 4×4 matrix, which are given as:

$$m=\begin{pmatrix}(L_1,L_1) & (L_1,L_2)\\ (L_2,L_1) & (L_2,L_2)\end{pmatrix}$$

$$k=\begin{pmatrix}(\nabla L_1,\nabla L_1) & (\nabla L_1,\nabla L_2)\\ (\nabla L_2,\nabla L_1) & (\nabla L_2,\nabla L_2)\end{pmatrix}$$

The calculation of numerical integration in the discrete model is the same as A1.2 so that the full discrete equation can be obtained as before

$$\begin{bmatrix}M+\Delta t\beta D\cdot K & -\Delta t\beta(1-\beta)R\cdot K\\ K & M\end{bmatrix}\begin{bmatrix}Q\\ P\end{bmatrix}^{t+1}=\begin{bmatrix}M & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}Q\\ P\end{bmatrix}^{t}$$

Here, $Q=\left[q^1,q^2\cdots q^n,q^{n+1}\right]$, $P=\left[p^1,p^2,\cdots,p^n,p^{n+1}\right]$, M and K are the mass matrix and stiffness matrix in the original domain, respectively.

If all coefficients in the model are functions of time, but independent of the spatial variables, the discrete formulation for the model on the spatial domain is the same as the case where all coefficients are constant. For the time integration the difference is that all coefficients have to be evaluated at each time step. With the new values the calculation is performed similarly to the case where the coefficients are constant. So that the full discrete equation is similar as before except that all coefficients have to be actualized at each time. Next, we will consider the numerical method with the coefficient depending on the spatial variables.

A5 Coefficients depending on the spatial variables for anisotropic domain.

We will consider the problem in R^2. The one dimensional case is a particular case. The solution concerns the case of no flux boundary conditions as previously. The Hermite finite element method with the BSF element will be used. A special case is studied where the reactivity coefficient $R=R(x,y)$ is function of the spatial variables and the fraction $\beta=\beta(R)$ depends on R. The diffusion coefficient D is constant.

Since the coefficient R associated with the domain R can be written as $R(x,y)$ consequrntly $\beta=\beta(R)$ can be written as $\beta(x,y)$. According to the bi-flux theory and the mass conservation principle, the equation can be written as below:

$$\int_V \frac{q(\mathbf{x},t+\Delta t)-q(\mathbf{x},t)}{\Delta t}\,ds+\int_{\partial V}\left[\beta\boldsymbol{\Psi}_1+(1-\beta)\boldsymbol{\Psi}_2^i\right]\cdot\left[\mathbf{e}_x,\mathbf{e}_y\right]ds=0 \qquad \text{(A-8)}$$

$$\mathrm{i}=1,2,3$$

Where the first flux $\boldsymbol{\Psi}_1=-D\nabla q(x,y,t)$ is defined according to the Fick's law. Depending on the position of $\beta(x,y)$ in the secondary flux potential equation, there are three possible alterantives:

$$\boldsymbol{\Psi}_2^1=R(x,y)\beta\nabla(\Delta q(x,y,t))$$

$$\boldsymbol{\Psi}_2^2=R(x,y)\nabla(\beta\Delta q(x,y,t))$$

$$\boldsymbol{\Psi}_2^3=R(x,y)\nabla(\nabla\cdot(\beta\nabla q(x,y,t)))$$

In the following it is shown the derivation of the mass matrix and the stiffness matrix with the material coeffcients depending on x and y. After actualization of the matrices at each time step the computation process is similar to the case of constant coeffcients.

Type I

The original model will be written as:

$$\frac{\partial q(\mathbf{x},t)}{\partial t}=\nabla(\beta D\nabla q(\mathbf{x},t))-\nabla(\beta(1-\beta)R\nabla(\Delta q(\mathbf{x},t))) \qquad \text{(A-9a)}$$

$$q(\mathbf{x},0)=q_0(\mathbf{x}),\ \mathbf{x}\in\Omega; \qquad \text{(A-9b)}$$

$$\nabla q(\mathbf{x},t)=0,\nabla^3 q(\mathbf{x},t)=0,\ \mathbf{x}\in\partial\Omega \qquad \text{(A-9c)}$$

The week formulation under the Galerkin method with Hermite element given as:

$$\int_\Omega \frac{\partial q(\mathbf{x},t)}{\partial t}\omega d\mathbf{x}=\int_\Omega(\nabla(\beta D\nabla q(\mathbf{x},t))-\nabla(\beta(1-\beta)R\nabla(p(\mathbf{x},t)))\ )\omega d\mathbf{x}$$

$$\int_\Omega \Delta q(\mathbf{x},t)\omega d\mathbf{x}=\int_\Omega p(\mathbf{x},t)\omega d\mathbf{x}$$

The mass matrix in the reference domain defined as:

$$m=\left(BS_{ij}, BS_{st}\right)=\int_{-1}^{1}\int_{-1}^{1} BS_{ij}\cdot BS_{st}\, d\xi d\eta$$

$$k=\left(\nabla BS_{ij}, \nabla BS_{ij}\right)=\int_{-1}^{1}\int_{-1}^{1} \frac{\partial BS_{ij}}{\partial\xi}\cdot\frac{\partial BS_{st}}{\partial\xi}+\frac{\partial BS_{ij}}{\partial\eta}\frac{\partial BS_{st}}{\partial\eta}\, d\xi d\eta\,,$$

$$k_{\beta}=\left(\beta(x,y)\nabla BS_{ij}, \nabla BS_{ij}\right)=\int_{-1}^{1}\int_{-1}^{1}\beta(x,y)\left(\frac{\partial BS_{ij}}{\partial\xi}\cdot\frac{\partial BS_{st}}{\partial\xi}+\frac{\partial BS_{ij}}{\partial\eta}\frac{\partial BS_{st}}{\partial\eta}\right)d\xi d\eta$$

$$k_{\beta R}=\left(\beta(1-\beta)R\nabla BS_{ij}, \nabla BS_{ij}\right)=\int_{-1}^{1}\int_{-1}^{1}\beta(x,y)(1-\beta(x,y))R(x,y)\left(\frac{\partial BS_{ij}}{\partial\xi}\cdot\frac{\partial BS_{st}}{\partial\xi}+\frac{\partial BS_{ij}}{\partial\eta}\frac{\partial BS_{st}}{\partial\eta}\right)d\xi d\eta$$

$$i=1,\ldots,4\,,\ j=1,\ldots,4\,,\ s=1,\ldots,4\,,\ t=1,\ldots,4$$

The semi-discrete formulation:

$$M\dot{Q}=D\cdot K_{\beta}Q+K_{\beta R}P$$

$$KQ+MP=0$$

$$Q=\left[q^{1}, q_{x}^{1}, q_{y}^{1}, q_{xy}^{1}\cdots, q^{n+1}, q_{x}^{n+1}, q_{y}^{n+1}, q_{xy}^{n+1}\right],$$

$$P=\left[p^{1}, p_{x}^{1}, p_{y}^{1}, p_{xy}^{1}\cdots, p^{n+1}, p_{x}^{n+1}, p_{y}^{n+1}, p_{xy}^{n+1}\right]$$

M , K , K_{β} , $K_{\beta R}$ are the mass matrix, stiffness matrix, stiffness matrix corresponding to β , stiffness matrix corresponding to β and R , in the original domain.

The full discrete formulation in matrix scheme

$$\begin{bmatrix} M+\Delta tDK_{\beta} & -\Delta tK_{\beta R} \\ K & M \end{bmatrix}\begin{bmatrix} Q \\ P \end{bmatrix}^{t+1}=\begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} Q \\ P \end{bmatrix}^{t} \qquad \text{(A-10)}$$

$$Q=\left[q^{1}, q_{x}^{1}, q_{y}^{1}, q_{xy}^{1}\cdots, q^{n+1}, q_{x}^{n+1}, q_{y}^{n+1}, q_{xy}^{n+1}\right],$$

$$P=\left[p^{1}, p_{x}^{1}, p_{y}^{1}, p_{xy}^{1}\cdots, p^{n+1}, p_{x}^{n+1}, p_{y}^{n+1}, p_{xy}^{n+1}\right]$$

M and K are the mass matrix and stiffness matrix in the original domain, respectively.

Type II

The original model will be written as:

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = \nabla(\beta D \nabla q(\mathbf{x},t)) - \nabla((1-\beta)R\nabla(\beta \Delta q(\mathbf{x},t))) \tag{A-11a}$$

$$q(\mathbf{x},0) = q_0(\mathbf{x}),\ \mathbf{x} \in \Omega; \tag{A-11b}$$

$$\nabla q(\mathbf{x},t) = 0\,, \nabla(\beta \Delta q(\mathbf{x},t)) = 0,\ \mathbf{x} \in \partial\Omega \tag{A-11c}$$

The week formulation under the Galerkin method with Hermite element is :

$$\int_\Omega \Delta q(\mathbf{x},t)\omega d\mathbf{x} = \int_\Omega \frac{1}{\beta} p(\mathbf{x},t)\omega d\mathbf{x}$$

$$\int_\Omega \frac{\partial q(\mathbf{x},t)}{\partial t}\omega d\mathbf{x} = \int_\Omega (\nabla(\beta D \nabla q(\mathbf{x},t)) - \nabla((1-\beta)R\nabla(p(\mathbf{x},t)))\ )\omega d\mathbf{x}$$

The mass matrix in the reference domain is defined as:

$$m = (BS_{ij}, BS_{st}) = \int_{-1}^{1}\int_{-1}^{1} BS_{ij} \cdot BS_{st} d\xi d\eta$$

$$m_\beta = (1/\beta(x,y)BS_{ij}, BS_{st}) = \int_{-1}^{1}\int_{-1}^{1} 1/\beta(x,y)BS_{ij} \cdot BS_{st} d\xi d\eta$$

$$k = (\nabla BS_{ij}, \nabla BS_{ij}) = \int_{-1}^{1}\int_{-1}^{1} \frac{\partial BS_{ij}}{\partial \xi} \cdot \frac{\partial BS_{st}}{\partial \xi} + \frac{\partial BS_{ij}}{\partial \eta}\frac{\partial BS_{st}}{\partial \eta} d\xi d\eta\,,$$

$$k_\beta = (\beta(\xi,\eta)\nabla BS_{ij}, \nabla BS_{ij}) = \int_{-1}^{1}\int_{-1}^{1} \beta(\xi,\eta)\left(\frac{\partial BS_{ij}}{\partial \xi} \cdot \frac{\partial BS_{st}}{\partial \xi} + \frac{\partial BS_{ij}}{\partial \eta}\frac{\partial BS_{st}}{\partial \eta}\right) d\xi d\eta$$

$$k_R = ((1-\beta)R\nabla BS_{ij}, \nabla BS_{ij}) = \int_{-1}^{1}\int_{-1}^{1} (1-\beta(\xi,\eta))R(\xi,\eta)\left(\frac{\partial BS_{ij}}{\partial \xi} \cdot \frac{\partial BS_{st}}{\partial \xi} + \frac{\partial BS_{ij}}{\partial \eta}\frac{\partial BS_{st}}{\partial \eta}\right) d\xi d\eta$$

$$i = 1,\ldots,4\,,\ j = 1,\ldots,4\,, s = 1,\ldots,4\,, t = 1,\ldots,4$$

The semi-discrete formulation:

$$M\dot{Q} = -D \cdot K_\beta Q + K_R P$$

$$KQ + M_\beta P = 0$$

$$Q = \left[q^1, q_x^1, q_y^1, q_{xy}^1 \cdots, q^{n+1}, q_x^{n+1}, q_y^{n+1}, q_{xy}^{n+1}\right]$$

and

$$P = \left[p^1, p_x^1, p_y^1, p_{xy}^1 \cdots, p^{n+1}, p_x^{n+1}, p_y^{n+1}, p_{xy}^{n+1}\right].$$

The full discrete formulation in matrix scheme

$$\begin{bmatrix} M + \Delta t K_\beta & -\Delta t K_R \\ K & M_\beta \end{bmatrix} \begin{bmatrix} Q \\ P \end{bmatrix}^{t+1} = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q \\ P \end{bmatrix}^{t} \tag{A-12}$$

$$Q = \left[q^1, q_x^1, q_y^1, q_{xy}^1 \cdots, q^{n+1}, q_x^{n+1}, q_y^{n+1}, q_{xy}^{n+1}\right],$$

$$P = \left[p^1, p_x^1, p_y^1, p_{xy}^1 \cdots, p^{n+1}, p_x^{n+1}, p_y^{n+1}, p_{xy}^{n+1}\right],$$

M, M_β, K, K_β, K_R are the mass matrix, mass matrix corresponding with β, stiffness matrix, stiffness matrix corresponding to β, stiffness matrix corresponding to β and R in the original domain.

Type III

The original model could be written as:

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = \nabla(\beta D \nabla q(\mathbf{x},t)) - \nabla \cdot ((1-\beta) R \nabla(\nabla \cdot (\beta \nabla q(\mathbf{x},t)))) \tag{A-13a}$$

$$q(\mathbf{x},0) = q_0(\mathbf{x}),\ \mathbf{x} \in \Omega; \tag{A-13b}$$

$$\nabla q(\mathbf{x},t) = 0,\ \nabla(\nabla \cdot (\beta \nabla q(\mathbf{x},t))) = 0,\ \mathbf{x} \in \partial\Omega \tag{A-13c}$$

The week formulation under the Galerkin method with Hermite element is:

$$\int_\Omega \frac{\partial q(\mathbf{x},t)}{\partial t} \omega d\mathbf{x} = \int_\Omega (\nabla \cdot (\beta D \nabla q(\mathbf{x},t)) - \nabla \cdot ((1-\beta) R \nabla(p(\mathbf{x},t)))\ ) \omega d\mathbf{x}$$

$$\int_\Omega \nabla \cdot (\beta \nabla q(\mathbf{x},t)) \omega d\mathbf{x} = \int_\Omega p(\mathbf{x},t) \omega d\mathbf{x}$$

The mass matrix in the reference domain is defined as:

$$m = \left(BS_{ij}, BS_{st}\right) = \int_{-1}^{1}\int_{-1}^{1} BS_{ij} \cdot BS_{st} d\xi d\eta$$

$$k = \left(\nabla BS_{ij}, \nabla BS_{ij}\right) = \int_{-1}^{1}\int_{-1}^{1} \frac{\partial BS_{ij}}{\partial \xi} \cdot \frac{\partial BS_{st}}{\partial \xi} + \frac{\partial BS_{ij}}{\partial \eta} \frac{\partial BS_{st}}{\partial \eta} d\xi d\eta ,$$

$$k_{\beta} = \left(\beta(\xi,\eta)\nabla BS_{ij}, \nabla BS_{ij}\right) = \int_{-1}^{1}\int_{-1}^{1} \beta(\xi,\eta)\left(\frac{\partial BS_{ij}}{\partial \xi} \cdot \frac{\partial BS_{st}}{\partial \xi} + \frac{\partial BS_{ij}}{\partial \eta} \frac{\partial BS_{st}}{\partial \eta} \right) d\xi d\eta$$

$$k_{R} = \left((1-\beta)R\nabla BS_{ij}, \nabla BS_{ij}\right) = \int_{-1}^{1}\int_{-1}^{1} (1-\beta(\xi,\eta))R(\xi,\eta)\left(\frac{\partial BS_{ij}}{\partial \xi} \cdot \frac{\partial BS_{st}}{\partial \xi} + \frac{\partial BS_{ij}}{\partial \eta} \frac{\partial BS_{st}}{\partial \eta} \right) d\xi d\eta$$

$$i = 1,\ldots,4 ,\ j = 1,\ldots,4 ,\ s = 1,\ldots,4 ,\ t = 1,\ldots,4$$

The semi-discrete formulation:

$$M\dot{Q} = D \cdot K_{\beta} Q + K_{R} P$$

$$K_{\beta} Q + MP = 0$$

$$Q = \left[q^{1}, q_{x}^{1}, q_{y}^{1}, q_{xy}^{1} \cdots, q^{n+1}, q_{x}^{n+1}, q_{y}^{n+1}, q_{xy}^{n+1}\right] \text{ and}$$
$$P = \left[p^{1}, p_{x}^{1}, p_{y}^{1}, p_{xy}^{1} \cdots, p^{n+1}, p_{x}^{n+1}, p_{y}^{n+1}, p_{xy}^{n+1}\right].$$

The full discrete formulation in matrix scheme

$$\begin{bmatrix} M + \Delta t K_{\beta} & -\Delta t K_{R} \\ K_{\beta} & M \end{bmatrix} \begin{bmatrix} Q \\ P \end{bmatrix}^{t+1} = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q \\ P \end{bmatrix}^{t} \qquad \text{(A-14)}$$

$$Q = \left[q^{1}, q_{x}^{1}, q_{y}^{1}, q_{xy}^{1} \cdots, q^{n+1}, q_{x}^{n+1}, q_{y}^{n+1}, q_{xy}^{n+1}\right] ,$$

$$P = \left[p^{1}, p_{x}^{1}, p_{y}^{1}, p_{xy}^{1} \cdots, p^{n+1}, p_{x}^{n+1}, p_{y}^{n+1}, p_{xy}^{n+1}\right],$$

M , K , K_{β} , K_{R} are the mass matrix, stiffness matrix, stiffness matrix corresponding to β , stiffness matrix corresponding with β and R , in the original domain.

B Numerical scheme for systems with *R* varying with the diffusion law

B1. *R* varies according to the diffusion law

In this section we will derive the numerical solution for a system where R varies according to a diffusion law**.** Assume the system as below, $\mathbf{x} \in R^2$:

$$\frac{\partial R(\mathbf{x},t)}{\partial t} = D_R \Delta R(\mathbf{x},t) \tag{B-1a}$$

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = \nabla(\beta D \nabla q(\mathbf{x},t)) - \nabla(\beta(1-\beta)R\nabla(\Delta q(\mathbf{x},t))) \tag{B-1b}$$

$$R(\mathbf{x},0) = R_0(\mathbf{x}) \ , \ \mathbf{x} \in \Omega \tag{B-1c}$$

$$q(\mathbf{x},0) = q_0(\mathbf{x}), \ \mathbf{x} \in \Omega \tag{B-1d}$$

$$\nabla R(\mathbf{x},t) = 0, \ \ \mathbf{x} \in \partial\Omega \tag{B-1e}$$

$$\nabla q(\mathbf{x},t) = 0 \, , \nabla^3 q(\mathbf{x},t) = 0 \, , \ \mathbf{x} \in \partial\Omega \tag{B-1f}$$

Suppose β and R are related as given below:

$$\beta = \exp(-\alpha \frac{R^2}{R_0^2})$$

Where R_0 is the maximum value for $R_0(\mathbf{x})$ on the domain at the initial time Let $\Delta q(\mathbf{x},t) = p(\mathbf{x},t)$. Substitute this expression in Eq.(B-1b,1f) to get:

$$\frac{\partial R(\mathbf{x},t)}{\partial t} = D_R \Delta R(\mathbf{x},t) \tag{B-2a}$$

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = \nabla(\beta D \nabla q(\mathbf{x},t)) - \nabla(\beta(1-\beta)R\nabla(p(\mathbf{x},t))) \tag{B-2b}$$

$$\Delta q(\mathbf{x},t) = p(\mathbf{x},t) \tag{B-2c}$$

$$R(\mathbf{x},0) = R_0(\mathbf{x}) \ , \ \mathbf{x} \in \Omega \tag{B-2d}$$

$$q(\mathbf{x},0)=q_0(\mathbf{x}),\ \mathbf{x}\in\Omega \tag{B-2e}$$

$$\nabla R(\mathbf{x},t)=0,\ \mathbf{x}\in\partial\Omega \tag{B-2f}$$

$$\nabla q(\mathbf{x},t)=0,\ \nabla p(\mathbf{x},t)=0\ ,\ \mathbf{x}\in\partial\Omega \tag{B-2g}$$

Let us call the computational domain Ω, $V=H^1(\Omega)$, $H=L^2(\Omega)$. Let us define the following norms related to the spaces V and H respectively:

$$(\phi,\varphi)=\int_\Omega \phi\cdot\varphi d\Omega$$

$$(\nabla\phi,\nabla\varphi)=\int_\Omega \nabla\phi\cdot\nabla\varphi d\Omega$$

Assume that V_h is the finite dimensional subspace of V. The Galerkin finite method for system (B-2) is to find $R_h, q_h, p_h \in V_h$, such that:

$$\frac{d(R_h,\omega)}{dt}+D_R(\nabla R_h,\nabla\omega)=0,\ \forall\omega\in V_h \tag{B-3a}$$

$$\frac{d(q_h,\omega)}{dt}+D(\beta\nabla q_h,\nabla\omega)-(\beta(1-\beta)R_h\nabla p_h,\nabla\omega)=0,\ \forall\omega\in V_h \tag{B-3b}$$

$$(p_h,\omega)+(\nabla q_h,\nabla\omega)=0\ ,\ \forall\omega\in V_h \tag{B-3c}$$

For time integration, we can see that in equation (B-3a), the only varaible is R. So that the strategy is first to solve the equation (B-3a), second to obtain the solution for q and p subject to the equation (B-3b) and (B-2c) using the same approach for R solved in (B-3a). The Euler backward difference is employed for time integration of the discrete equations.

In the sequel it is shown the process of implementation of the Galerkin finite element method with BSF element.

Denote the same symbols M and K as the global mass matrix and global stiffness matrix in the original domain, and m, k the local mass matrix and local stiff matrix, respectively.

The full discrete scheme for (B-3a) using the Euler backward difference written in matrix notation is:

$$[M+\Delta t D_R K]R^{n+1}=MR^n \tag{B-4}$$

Here, for simplicity of notation let us call $R=\left[R^1, R_x^1, R_y^1, R_{xy}^1 \cdots, R^{n+1}, R_x^{n+1}, R_y^{n+1}, R_{xy}^{n+1}\right]$, which means the value of R at each point of the mesh. Under the computation platform Matlab, the solution for (B-4) can be obtained.

Then the solution R from the equation (B-2a) may be written as:

$$R_h(x,y)=\sum_{j=1}^{ns} BS_{j1}(x,y)q_1^j + BS_{j2}(x,y)q_2^j h_x + BS_{j3}(x,y)q_3^j h_y + BS_{j4}(x,y)q_4^j h_x h_y$$

Let BS_{ji}, $j=1,...ns$, $i=1,...4$ be the base functions in the original domain, with ns indicating the number of the element.

For the system (B-3b) and (B-3c), the full discrete matrix equation can be written as:

$$\begin{bmatrix} M+\Delta t D\cdot K_\beta & -\Delta t K_{\beta R} \\ K & M \end{bmatrix}\begin{bmatrix} Q \\ P \end{bmatrix}^{t+1} = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} Q \\ P \end{bmatrix}^{t} \qquad \text{(B-5)}$$

where

$$Q=\left[q^1, q_x^1, q_y^1, q_{xy}^1 \cdots, q^{n+1}, q_x^{n+1}, q_y^{n+1}, q_{xy}^{n+1}\right],$$

$$P=\left[p^1, p_x^1, p_y^1, p_{xy}^1 \cdots, p^{n+1}, p_x^{n+1}, p_y^{n+1}, p_{xy}^{n+1}\right],$$

M, K, K_β, $K_{\beta R}$ are the mass matrix, stiffness matrix, stiffness matrix corresponding to β, stiffness matrix corresponding to β and R, on the original domain. (B-5) is similar to the full discrete equation (A-10) obtained in A2.1. But, in (B-5)

$$k_\beta=\left(\beta(x,y)\nabla BS_{ij}, \nabla BS_{ij}\right)=\int_{-1}^{1}\int_{-1}^{1}\beta(R_h)\left(\frac{\partial BS_{ij}}{\partial \xi}\cdot\frac{\partial BS_{st}}{\partial \xi}+\frac{\partial BS_{ij}}{\partial \eta}\frac{\partial BS_{st}}{\partial \eta}\right)d\xi d\eta$$

$$k_{\beta R}=\left(\beta(1-\beta)R_h\nabla BS_{ij}, \nabla BS_{ij}\right)=\int_{-1}^{1}\int_{-1}^{1}\beta(R_h)(1-\beta(R_h))R_h\left(\frac{\partial BS_{ij}}{\partial \xi}\cdot\frac{\partial BS_{st}}{\partial \xi}+\frac{\partial BS_{ij}}{\partial \eta}\frac{\partial BS_{st}}{\partial \eta}\right)d\xi d\eta$$

$$i=1,...,4,\ j=1,...,4,\ s=1,...,4,\ t=1,...,4$$

B2. *R* varies according to the diffusion law with source

Let us consider now the case where the reactivity coefficient R follows the classical diffusion law with a source. Consider the system below, $\mathbf{x} \in R^2$:

$$\frac{\partial R(\mathbf{x},t)}{\partial t} = D_R \Delta R(\mathbf{x},t) + A \cdot R(\mathbf{x},t) \tag{B-6a}$$

$$\frac{\partial q(\mathbf{x},t)}{\partial t} = \nabla(\beta D \nabla q(\mathbf{x},t)) - \nabla(\beta(1-\beta) R \nabla(\Delta q(\mathbf{x},t))) \tag{B-6b}$$

$$R(\mathbf{x},0) = R_0(\mathbf{x}) \text{ , } \mathbf{x} \in \Omega \tag{B-6c}$$

$$q(\mathbf{x},0) = q_0(\mathbf{x}), \ \mathbf{x} \in \Omega \tag{B-6d}$$

$$\nabla R(\mathbf{x},t) = 0, \ \ \mathbf{x} \in \partial\Omega \tag{B-6e}$$

$$\nabla q(\mathbf{x},t) = 0 \,, \nabla^3 q(\mathbf{x},t) = 0 \,, \ \mathbf{x} \in \partial\Omega \tag{B-6f}$$

Let A be constant. The process is the same comparing with (B-1) except that the semi-discrete equation (B-4) need to be written as:

$$\left[M - \Delta t A M + \Delta t D_R K\right] R^{n+1} = M R^n \tag{B-7}$$

From this equation, the numerical solution for R on each point and time of the mesh grid could be obtained. The procedure then follows the same steps as for the previous case corresponding to the system (B-5). The numerical solutions for are performed, using the platform Matlab.

C Numerical scheme for bi-flux model with nonlinear source or sink

C1 Model with the Dirichlet boundary condition

We will consider our new fourth order equation in two dimensions with source or sink term as shown below.

$$\frac{\partial q(x,y,t)}{\partial t} = \nabla \cdot (\beta D \nabla q(x,y,t)) - \nabla \cdot (\beta(1-\beta) R \nabla(\Delta q(x,y,t))) + q - q^3$$

$$\forall (x,y) \in \Omega$$

Subject to the boundary condition:

$$q(x,y) = 0\,;\Delta q(x,y) = 0\,.\ \forall (x,y) \in \partial\Omega$$

The equation will be called as the extended Fisher-Kolmogorov (EFK) equation. A nonlinear Galerkin finite element method will be presented in this part, that will be used to obtain the numerical solution for the flux q(x,t) with the Hermite base function.

The original nonlinear Galerkin method idea is from Marion and Temam, (1989). In this part, we will consider the computational domain as Ω, the space $V = H_0^1(\Omega)$, and $H = L^2(\Omega)$. There are several definitions of the scalar products and norms are:

$$(\phi,\varphi) = \int_\Omega \phi \cdot \varphi d\Omega\,,\ \|\phi\|_{L^2} = (\phi,\phi)^{\frac{1}{2}},\ \forall \phi,\varphi \in H\ .$$

$$(\nabla\phi,\nabla\varphi) = \int_\Omega \nabla\phi \cdot \nabla\varphi d\Omega\,,\ \|\nabla\phi\|_{L^2} = (\nabla\phi,\nabla\phi)^{\frac{1}{2}},\ \forall \phi,\varphi \in H$$

$$(\nabla^2\phi,\nabla^2\varphi) = \int_\Omega \nabla^2\phi \cdot \nabla^2\varphi d\Omega\,,\ \|\nabla^2\phi\|_{L^2} = (\nabla^2\phi,\nabla^2\phi)^{\frac{1}{2}},\ \forall \phi,\varphi \in H$$

Assume that V_h is a finite dimensional subspace of V. First, considering the classical Fisher- Kolmogorov model and employing the variational principle for the classical model.

$$\frac{\partial q(x,y,t)}{\partial t} = D\Delta q(x,y,t) + q - q^3$$

we can obtain the classical Galerkin expression to find $q_h \in V_h$ such that:

$$\frac{d}{dt}(q_h,\phi) + D(\nabla q_h,\nabla\phi) = (F(q_h),\phi),\ \forall \phi \in V_h$$

For 1D case, the nonlinear Galerkin method proposed in previous paper (Marion and Temam, 1989, 1990), two levels of discretization V_{2h} and W_h are considered, V_{2h} with the mesh parameter $2h$ and W_h twice finer with respect to mesh parameter h. The subspace V_{2h} consist of the nodal (hat) function $\phi_{j,2h}$ that are equal to 1 at $2jh(j=0,...,N)$ and are equal to 0 at the other nodes $2kh(k=0,...,N,k \neq j)$. The other subspace W_h consists of the nodal (hat) function $\varphi_{j,2h}$ whose values are equal to 1 at the nodes $2(j+1)h(j=0,...,N)$ and are equal to 0 at the other nodes $kh(k=0,...,N2,k \neq 2j+1)$. The union of bases function of V_{2h} and W_h yields a basis of V_h which is not the canonical nodal basis of V_h. This hierarchical basis is obtained by refining the mesh, so we call it h-type hierarchical basis.

Another kind of hierarchical basis function is called p-type hierarchical basis which is showed in paper (Zhang *et al.*,2016). Consider two spaces V_l and V_q, such that V_l corresponds to a space associated with lower-degree shape functions, while V_q corresponds to a space associated with high-degree shape function. The union of two spaces V_l and V_q yields a space V_h in which the hierarchical basis is represented as one combination of lower-degree base function and high-degree base function.

Let us recall the idea of this kind of base function. They are quadratic or high order correction as compared with the order of base polynomial in rough grid. Here, the quadratic correction is referred to the linear shape function over an element. The subspace V_l consists of the nodal (hat) function ϕ_j that are equal 1 at $jh(j=0,...,N)$ and are equal to 0 for the other nodal (hat) function ϕ_k $kh(j=0,...,N,k \neq j)$. And the other subspace V_q consists of quadratic hierarchical shape function on each element. This quadratic function, $\varphi_j \in V_q(j=1,...,N)$, to a canonical element $\xi = 2(x-x_j)/h \in [-1,1]$ has the form:

$$\varphi_j(\xi) = 1-\xi^2$$

As the same theory about p-type hierarchical basis function, we will consider for the Hermite base function, for instance, reference interval given as [-1,1], the Herimte base function given $\phi_1(\xi)=0.25(2-3\xi+\xi^3)$, with $\phi_1(-1)=1$ and $\phi_1(1)=0$, the first derivate at the point 1 and -1 are equal 0 as well, with the notation $\phi_1'(-1)=\phi_1'(1)=0$; $\phi_2(\xi)=0.25(1-\xi-\xi^2+\xi^3)$, with the first derivate at the point -1 equal to 1, also $\phi_2'(-1)=1$, and $\phi_2(-1)=\phi_2(1)=\phi_2'(1)=0$; $\phi_3(\xi)=0.25(2+3\xi-\xi^3)$, that at the point 1 gives, $\phi_3(1)=1$ and $\phi_3(-1)=\phi_3'(1)=\phi_3'(-1)=0$; $\phi_4(\xi)=0.25(-1-\xi+\xi^2+\xi^3)$, that at the point 1 gives, $\phi_4'(1)=1$and $\phi_4(-1)=\phi_4(1)=\phi_4'(-1)=0$. The first kind of high-degree correction base function requires that in the middle of the reference point the value of the function is 1, the first derivate is zero, and its value and first derivate value at the left and right point are zero. Under these six conditions, we will obtain the "six order" polynomial, but unfortunately, the coefficients for the sixth and fifth order are zero as written as below:

$$\varphi_1(\xi)=1-2\xi^2+\xi^4$$

The second kind of high-degree correction base function correspond to the condition that in the middle of the reference point the value of the function is zero, the first derivate is one, and its value and first derivate value at the left and right point will be zero. Under these six conditions, the "six order" polynomial in the sequel can be obtained, but unfortunately, the coefficient for the sixth is zero as can be seen form the definition written as below:

$$\varphi_2(\xi)=\xi-2\xi^3+\xi^5$$

Consider now the bi-flux theory. The following variational principle and classical Galerkin method for the bi-flux theory will be introduced to find $q_h \in V_h$ such that

$$\frac{d}{dt}(q_h,\phi)+D\beta(\nabla q_h,\nabla\phi)+\beta(1-\beta)R\left(\nabla^2 q_h,\nabla^2\phi\right)=\left(F(q_h),\phi\right),\ \forall\phi\in V_h$$

With the nonlinear Galerkin method (Marion and Temam, 1989, 1990, 1995), we will write the approximation in the form:

$$q_h(t)=q_l(t)+q_q(t),\ \ q_l(t)\in V_l,\ q_q(t)\in V_q$$

Such that

$$\frac{d}{dt}(q_l,\phi)+D\beta(\nabla q_h,\nabla\phi)+\beta(1-\beta)R\left(\nabla^2 q_h,\nabla^2\phi\right)=\left(F(q_h),\phi\right)$$

$$D\beta(\nabla q_h,\nabla\varphi)+\beta(1-\beta)R\left(\nabla^2 q_h,\nabla^2\varphi\right)=\left(F(q_h),\varphi\right)$$

$$(q_h(0),\phi)=(q_0,\phi)$$

In this case, we can't find two different orthogonal subspaces such that the scalar products for the base functions vanish, therefore the simple formula as in the paper

(Nabh *et al.*, 1996; Dubois *et al.*,, 1998, 1999, 2004) can’t be found. For the nonlinear term in the right hand side, we will consider for a simple discrete approximation:

$$\left(F\left(q_h\right),\varphi\right)=\left(F\left(q_l\right)+F'\left(q_l\right)z_h,\varphi\right)$$

Where $F'\left(q_l\right)$ is the Jacobian matrix. For the sake of computation, we will write the formula in matrix notation:

$$\frac{d}{dt}\left(Q_l,\Phi\right)+D\beta\left(\nabla\left(Q_l+Z_q\right),\nabla\Phi\right)+\beta(1-\beta)R\left(\nabla^2\left(Q_l+Z_q\right),\nabla^2\Phi\right)=\left(F\left(Q_l+Z_q\right),\Phi\right)$$

$$D\beta\left(\nabla\left(Q_l+Z_q\right),\nabla\Psi\right)+\beta(1-\beta)R\left(\nabla^2\left(Q_l+Z_q\right),\nabla^2\Psi\right)=\left(F\left(Q_l\right)+F'\left(Z_q\right)\Psi_q,\Psi\right)$$

$$\left(Q_l(0),\Phi\right)=\left(Q_0,\Phi\right)$$

Where $Q_l(t)=\sum_{k=0}^{N-1}\sum_{i=1}^{2}q_{4k+i}(t)\phi_{4k+i}$,

$Z_q(t)=\sum_{k=0}^{N-2}\sum_{i=1}^{2}z_{4k+2+i}(t)\varphi_{4k+2+i}$,

$\Phi=\left[\phi_1,\phi_2,\phi_5,\phi_6,\ldots,\phi_{4N-7},\phi_{4N-6},\phi_{4N-3},\phi_{4N-2}\right]'$,

$\Psi=\left[\varphi_3,\varphi_4,\phi_7,\phi_8,\ldots,\phi_{4N-11},\phi_{4N-10},\phi_{4N-7},\phi_{4N-6}\right]'$.

For time integration, the semi-implicit backward differentiation scheme will be employed for the equation, subsequently, the full discrete scheme can be written as:

$$\frac{\left(Q_l^{n+1},\Phi\right)}{dt}-\frac{\left(Q_l^{n},\Phi\right)}{dt}+D\beta\left(\nabla\left(Q_l^{n+1}+Z_q^{n+1}\right),\nabla\Phi\right)+\beta(1-\beta)R\left(\nabla^2\left(Q_l^{n+1}+Z_q^{n+1}\right),\nabla^2\Phi\right)=\left(F\left(\left(Q_l^{n+1}+Z_q^{n+1}\right)\right),\Phi\right)$$

$$D\beta\left(\nabla\left(\left(Q_l^{n}+Z_q^{n+1}\right)\right),\nabla\Psi\right)+\beta(1-\beta)R\left(\nabla^2\left(\left(Q_l^{n}+Z_q^{n+1}\right)\right),\nabla^2\Psi\right)=\left(F\left(Q_l^{n}\right)+F'\left(Z_q^{n+1}\right)\Psi_q,\Psi\right)$$

$$\left(Q_l^{1}(0),\Phi\right)=\left(Q_0,\Phi\right)$$

The solution could be obtained on each point and at each time step with the platform Matlab.

C2 Model with no flux boundary condition

In this section we consider the same model as C1 except that the boundary conditions correspond now to non-flux. The main fourth order equation is decoupled into two second order equations and the solution is obtained with the nonlinear Galerkin finite element on the interval [-1,1] for the spatial domain and the Euler backward difference method for the time integration. Due to the no flux boundary condition, the model is written as :

$$\frac{\partial q(x,t)}{\partial t} = \beta D \frac{\partial^2 q(x,t)}{\partial x^2} - \beta(1-\beta) R \frac{\partial^4 q(x,t)}{\partial x^4} + q - q^3$$

$$\frac{\partial q(-1,t)}{\partial x} = \frac{\partial q(1,t)}{\partial x} = 0\,; \frac{\partial q^3(-1,t)}{\partial x^3} = \frac{\partial q^3(1,t)}{\partial x^3} = 0$$

$$q(x,0) = q_0(x), \qquad x \in [-1,1]$$

Let $\partial^2 q(x,t)/\partial x^2 = p(x,t)$, the model rewritten as below:

$$\frac{\partial q(x,t)}{\partial t} = \beta D \frac{\partial^2 q(x,t)}{\partial x^2} - \beta(1-\beta) R \frac{\partial^2 p(x,t)}{\partial x^2} + q - q^3$$

$$\partial^2 q(x,t)/\partial x^2 = p(x,t)$$

$$\frac{\partial q(-1,t)}{\partial x} = \frac{\partial q(1,t)}{\partial x} = 0\,; \frac{\partial p(-1,t)}{\partial x} = \frac{\partial p(1,t)}{\partial x} = 0$$

$$q(x,0) = q_0(x), \qquad x \in [-1,1]$$

Let $V = H_0^1(I)$, and $H = L^2(I)$. $I = [-1,1]$. The definitions of the scalar products and norms in one dimension case are:

$$(\phi,\varphi) = \int_I \phi \cdot \varphi d\Omega\,,\ \|\phi\|_{L^2} = (\phi,\phi)^{\frac{1}{2}}\,,\ \forall \phi,\varphi \in H\ .$$

$$\left(\nabla\phi,\nabla\varphi\right)=\int_I\frac{\partial\phi}{\partial x}\cdot\frac{\partial\varphi}{\partial x}d\Omega\,,\ \left\|\nabla\phi\right\|_{L^2}=\left(\nabla\phi,\nabla\phi\right)^{\frac{1}{2}},\ \forall\phi,\varphi\in H$$

Assume that V_h is a finite dimensional subspace of V. Consider the classical Galerkin formula is to find $q_h, p_h \in V_h$ such that:

$$\frac{d}{dt}(q_h,\phi)+\beta D(\nabla q_h,\nabla\phi)-\beta(1-\beta)R(\nabla p_h,\nabla\phi)=\left(F(q_h),\phi\right)$$

$$\left(\nabla q_h,\nabla\phi\right)+\left(p_h,\phi\right)=0$$

Due to the nonlinear Galerkin method (Marion and Temam, 1989, 1990, 1995; Nabh *et al.,* 1996; Dubois *et al.,*, 1998, 1999, 2004; Dettori *et al.,*, 1995; Laminie *et al.,*,1993; García-Archilla *et al.,*, 1995; Zhang, 2016), we will split the solution into two parts:

$$q_h(t)=q_l(t)+q_q(t),\ \ q_l(t)\in V_l\,,\ q_q(t)\in V_q$$

$$p_h(t)=p_l(t)+p_q(t),\ \ p_l(t)\in V_l\,,\ p_q(t)\in V_q$$

to obtain:

$$\frac{d}{dt}(q_l,\phi)+D\beta(\nabla q_h,\nabla\phi)-\beta(1-\beta)R(p_h,\phi)=\left(F(q_h),\phi\right)$$

$$\left(\nabla q_h,\nabla\phi\right)+\left(p_h,\phi\right)=0$$

$$D\beta(\nabla q_h,\nabla\varphi)-\beta(1-\beta)R\left(\nabla^2 q_h,\nabla^2\varphi\right)=\left(F(q_h),\varphi\right)$$

$$\left(q_h(x,0),\phi\right)=\left(q_0,\phi\right)$$

$$\left(p_h(x,0),\phi\right)=\left(\Delta q_0(x,0),\phi\right)=\left(p_0,\phi\right)$$

Consider the same approach as in C1 for the nonlinear source or sink

$$\left(F(q_h),\varphi\right)=\left(F(q_l)+F'(q_l)z_h,\varphi\right)$$

Where $F'(q_l)$ is the Jacobian matrix. The system can now be written:

$$\frac{d}{dt}(Q_l,\Phi)+D\beta\left(\nabla\left(Q_l+Z_q\right),\nabla\Phi\right)-\beta(1-\beta)R\left(\left(P_l+U_q\right),\Phi\right)=\left(F\left(Q_l+Z_q\right),\Phi\right)$$

$$\left(\nabla\left(Q_l+Z_q\right),\nabla\Phi\right)+\left(\left(P_l+U_q\right),\Phi\right)=0$$

$$D\beta\left(\nabla\left(Q_l+Z_q\right),\nabla\Psi\right)-\beta(1-\beta)R\left(\left(P_l+U_q\right),\Psi\right)=\left(F\left(Q_l\right)+F'\left(Z_q\right)\Psi_q,\Psi\right)$$

$$\left(Q_l(0),\Phi\right)=\left(Q_0,\Phi\right)$$

$$\left(P_l(0),\Phi\right)=\left(P_0,\Phi\right)$$

Where $Q_l(t)=\sum_{k=0}^{N-1}q_{2k+1}(t)\phi_{2k+1}$,

$Z_q(t)=\sum_{k=0}^{N-2}z_{2k+2}(t)\varphi_{2k+2}$,

$P_l(t)=\sum_{k=0}^{N-1}p_{2k+1}(t)\phi_{2k+1}$,

$U_q(t)=\sum_{k=0}^{N-2}u_{2k+2}(t)\varphi_{2k+2}$

$\Phi=\left[\phi_1,\phi_3,\ldots,\phi_{2N-1},\phi_{2N+1}\right]'$,

$\Psi=\left[\varphi_2,\varphi_4,,\ldots,\phi_{2N-2},\phi_{2N}\right]'$.

For time integration the semi-implicit backward differentiation scheme will be employed, subsequently the full discrete scheme written for each time step as:

$$\frac{\left(Q_l^{n+1},\Phi\right)}{dt}-\frac{\left(Q_l^{n},\Phi\right)}{dt}+D\beta\left(\nabla\left(Q_l^{n+1}+Z_q^{n+1}\right),\nabla\Phi\right)-\beta(1-\beta)R\left(\left(P_l^{n+1}+U_q^{n+1}\right),\Phi\right)=\left(F\left(\left(Q_l^{n+1}+Z_q^{n+1}\right)\right),\Phi\right)$$

$$\left(\nabla\left(Q_l^{n+1}+Z_q^{n+1}\right),\nabla\Phi\right)+\left(\left(P_l^{n+1}+U_q^{n+1}\right),\Phi\right)=0$$

$$D\beta\left(\nabla\left(\left(Q_l^{n}+Z_q^{n+1}\right)\right),\nabla\Psi\right)-\beta(1-\beta)R\left(\left(P_l^{n}+U_q^{n+1}\right),\Psi\right)=\left(F\left(Q_l^{n}\right)+F'\left(Z_q^{n+1}\right)\Psi_q,\Psi\right)$$

$$\left(\nabla\left(Q_l^n + Z_q^{n+1}\right), \nabla\Phi\right) + \left(\left(P_l^n + U_q^{n+1}\right), \Phi\right) = 0$$

$$\left(Q_l^1(0), \Phi\right) = \left(Q_0, \Phi\right)$$

$$\left(P_l^1(0), \Phi\right) = \left(P_0, \Phi\right)$$

The solution could be obtained on the each point and time under the platform Matlab.

C3 Coupled model with no flux boundary condition

In this section, we will consider the Gray-Scott model with fourth order term called extended Gray-Scott model as below. The coefficients $\beta_q, \beta_v, D_q, D_v, R_q, R_v$ are constant.

$$\frac{\partial q(x,t)}{\partial t} = \beta_q D_q \frac{\partial^2 q(x,t)}{\partial x^2} - \beta_q \left(1-\beta_q\right) R_q \frac{\partial^4 q(x,t)}{\partial x^4} - qv^2 + A(1-q)$$

$$\frac{\partial v(x,t)}{\partial t} = \delta^2 \beta_v \frac{\partial^2 v(x,t)}{\partial x^2} - \beta_v \left(1-\beta_v\right) R_v \frac{\partial^4 v(x,t)}{\partial x^4} + qv^2 - Bv$$

$$\frac{\partial q(-1,t)}{\partial x} = \frac{\partial q(1,t)}{\partial x} = 0\,; \frac{\partial q^3(-1,t)}{\partial x^3} = \frac{\partial q^3(1,t)}{\partial x^3} = 0$$

$$\frac{\partial v(-1)}{\partial x} = \frac{\partial v(1)}{\partial x} = 0\,; \frac{\partial v^3(-1)}{\partial x^3} = \frac{\partial v^3(1)}{\partial x^3} = 0$$

$$q(x,0) = q_0(x),\ x \in [-1,1]$$

$$v(x,0) = v_0(x), x \in [-1,1]$$

The process to deal with this system is to expand the single variation developed in C2 into two variations for the present problem. The sequence of the solution is similar, so that we just list the last full discrete matrix formulation as :

$$\frac{(Q_l^{n+1},\Phi)}{dt}-\frac{(Q_l^{n},\Phi)}{dt}+\beta_q D_q(\nabla(Q_l^{n+1}+Z_q^{n+1}),\nabla\Phi)-\beta_q(1-\beta_q)R_q((P_l^{n+1}+U_q^{n+1}),\Phi)$$
$$=(F((Q_l^{n+1}+Z_q^{n+1},E_l^{n+1}+L_q^{n+1})),\Phi)$$
$$(\nabla(Q_l^{n+1}+Z_q^{n+1}),\nabla\Phi)+((P_l^{n+1}+U_q^{n+1}),\Phi)=0$$

$$\frac{(Q_l^{n+1},\Phi)}{dt}-\frac{(Q_l^{n},\Phi)}{dt}+\delta^2\beta_v(\nabla(V_l^{n+1}+T_q^{n+1}),\nabla\Phi)-\beta_v(1-\beta_v)R_v((E_l^{n+1}+L_q^{n+1}),\Phi)$$
$$=(G((Q_l^{n+1}+Z_q^{n+1},E_l^{n+1}+L_q^{n+1})),\Phi)$$
$$(\nabla(V_l^{n+1}+T_q^{n+1}),\nabla\Phi)+((E_l^{n+1}+L_q^{n+1}),\Phi)=0$$

$$\beta_q D_q(\nabla((Q_l^{n}+Z_q^{n+1})),\nabla\Psi)-\beta_q(1-\beta_q)R_q((P_l^{n}+U_q^{n+1}),\Psi)$$
$$=(F((Q_l^{n+1},E_l^{n+1}))+F_Q(Z_q^{n+1})\Psi_q+F_E(L_v^{n+1})\Psi_v,\Psi)$$

$$(\nabla(Q_l^{n}+Z_q^{n+1}),\nabla\Phi)+((P_l^{n}+U_q^{n+1}),\Phi)=0$$

$$\delta^2\beta_v(\nabla((V_l^{n}+T_q^{n+1})),\nabla\Psi)-\beta_v(1-\beta_v)R_v((E_l^{n}+L_q^{n+1}),\Psi)$$
$$=(G((Q_l^{n+1},E_l^{n+1}))+G_Q(Z_q^{n+1})\Psi_q+G_E(L_v^{n+1})\Psi_v,\Psi)$$

$$(\nabla(V_l^{n}+T_q^{n+1}),\nabla\Phi)+((E_l^{n}+L_q^{n+1}),\Phi)=0$$

$$(Q_l^1(0),\Phi)=(Q_0,\Phi)$$

$$(P_l^1(0),\Phi)=(P_0,\Phi)$$

$$(V_l^1(0),\Phi)=(V_0,\Phi)$$

$$(E_l^1(0),\Phi)=(E_0,\Phi)$$