A NUMERICAL SOLUTION OF THE DIFFUSION-RETENTION PROBLEM IN HOMOGENEOUS MEDIA

Augusto C.N.R.Galeão, acng@lncc.br
Luiz Bevilacqua, bevilacqua@coc.ufrj.br
Laboratório Nacional de Computação Científica, Petrópolis, RJ
Programa de Engenharia Civil, Instituto A.L.Coimbra, COPPE, UFRJ, Rio de Janeiro, RJ

Simone Delphin, delphin@lncc.br
Universidade Federal do Amapá, Macapá, AP

Flávio Pietrobon, pietrobon_costa@yahoo.com.br
Universidade Estadual de Santa Cruz, Ilhéus, BA

Abstract. This paper presents a new law for the diffusion-retention problem. The retention effect, which is assumed to be temporary, requires the introduction of a fourth order term in the governing equation. All particle need to be effective all time to avoid exchanging of energy with the surroundings. It is also introduced a control parameter that avoids the formation of "black holes" requiring that retention is only possible in the presence of diffusion. A variational formulation is introduced to generate a numerical approach based on a semi-discrete version of the Galerkin method. The results show clearly the time delay in the spreading process due to the retention effect.

Keywords. Diffusion, retention, numerical solutions, fourth order PDE

1. INTRODUCTION

The governing equation for the diffusion-retention problem was introduced in previous seminars and conferences. The fundamental law characterizing diffusion with temporary retention was introduced after the results obtained with the discrete approach formulation of a generalized population dynamics problem. If an invading population keeps part of its total number of individuals temporary stationary in order to colonize the occupied territory then it can be shown that the corresponding governing equation requires a fourth order differential term. That is to say that the fundamental equation for diffusion with temporary retention is a fourth order partial differential equation for the case of population dynamics.

The formulation of the diffusion-retention problem for the case of physic-chemical problems, provided that all particles remain in the process all time and a fraction of the particles is temporarily trapped, belongs to the same class of problems. A retention law was proposed by the first two authors that complements the Fick's law and leads to a new fundamental equation (Bevilacqua, Galeão, Costa, 2010). For the simple case of one-dimensional diffusion in an isotropic and homogeneous medium the generalized diffusion-retention law can be stated as follows:

1.The diffusion law follows the classical Fick's assumption, that is, the diffusion vector equals minus the gradient of the concentration function $p(x,t)$ multiplied by the diffusion coefficient D:

$$\vec{d} = -grad\big(Dp(x,t)\big) \qquad (1\text{-}a)$$

2.The retention law follows a concept similar to the diffusion law. The retention vector is proportional to the gradient of the second derivative of the concentration function with respect to the space variable x multiplied by the retention coefficient ρ:

$$\vec{b} = \beta grad\left(\rho \frac{\partial^2 p(x,t)}{\partial x^2} \right) \qquad (1\text{-}b)$$

The factor β is the fraction of the diffusing particles and works as a control parameter that may vary within the range [0,1]. It is also important to note that the vector $\vec{b}$ means the actual potentiality of the medium to retain the diffusing particles but not the effective fraction of retained particles. The effective fraction of particles trapped in the process is given by $(1-\beta)$. If $\beta=1$ there is no retention all particles are under a diffusion process. If $\beta=0$ all particles are retained and the solution degenerates into a stationary state. Equation (1-b) expresses the fundamental condition that retention is only possible in the presence of diffusion. There is no retention as an isolated phenomenon it is always coupled to the diffusion process. The dynamical process is accordingly controlled by the product $\beta (1-\beta)$ as indicated in the equation (2) below.

It is also important to recall that the retention as considered here is always a temporary phenomenon. This means that even when the fraction of the particles $(1-\beta)$ trapped in the medium remains constant they may not be the same all the time. All particles are active in the process, possibly jumping from the diffusion state to the retention state at random provided that the total fraction $(1-\beta)$ remains the same. It is also important to remark that there is no energy or work exchange with the surroundings as it should be if the process would be modeled by sources and sinks coming into play alternatively.

Several other approaches to deal with the retention effect in diffusion processes have been proposed all of them, to the best of our knowledge, introducing some correction terms in the classical second order partial differential equation, that one best adequated to the particular problem under consideration (D`Angelo , Fontana , Chertcoff , Rosen, 2003; Deleersnijder, Beckers, Delhez, 2006; Atsumi, 2002). Therefore these results lack the generality required for a more universal proposition.

2. GOVERNING EQUATION

With the diffusion-retention law stated above and recalling the conservation mass principle it is not difficult to derive the following equation for an isotropic homogeneous medium:

$$\frac{\partial p(x,t)}{\partial t} = -\rho \frac{\partial}{\partial x}\left[\beta(1-\beta)\frac{\partial^3 p(x,t)}{\partial x^3}\right] + D\frac{\partial}{\partial x}\left[\beta\frac{\partial p(x,t)}{\partial x}\right] \tag{2}$$

Clearly if $\beta=1$ the equation (2) reduces to the classical diffusion equation and if $\beta=0$ the problem falls into the case of retention only which is a trivial physic-chemical state. For the later case the system is reduced to a stationary state.

Now in general we may expect that the parameter β is not constant. Since we are assuming the medium to be homogeneous we may say that it is not an explicit function of x but it could be function of time and more likely of the concentration function $p(x,t)$. So in principle we may have a functional relation coupling β , $p(x,t)$ and possible the first derivative of $p(x,t)$ with respect to x:

$$\Im\left(\beta, p(x,t), \frac{\partial p(x,t)}{\partial x}\right) = 0 \tag{3}$$

The solution of the diffusion-retention problem is therefore complex since there is a coupling between $p(x,t)$ and β which behaves as a new independent variable. The functional relation (3) is not known. Theoretical and experimental research need to be fostered to determine the best approximation for the equation (3). The two simplest possibilities for the relation between $p(x,t)$ and β are either set β constant or assume the most elementary relation that is a linear function of the form:

$$\beta = \frac{p(x,t)}{p_0}$$

This means that there is a saturation limit p_0 for which retention stops and only diffusion is effective. With this definition for β and calling $q(x,t) = \beta = p(x,t)/p_0$ the equation (3) reads

$$\frac{\partial q}{\partial t} = D\left(\frac{\partial q}{\partial x}\right)^2 + Dq\frac{\partial^2 q}{\partial x^2} + \rho(-1+2q)\frac{\partial q}{\partial x}\frac{\partial^3 q}{\partial x^3} - \rho q(1-q)\frac{\partial^4 q}{\partial x^4} \tag{4-a}$$

For the simple case β = constant the equation (2) reduces to:

$$\frac{\partial p(x,t)}{\partial t} = D\beta \frac{\partial^2 p(x,t)}{\partial x^2} - \rho\beta(1-\beta)\frac{\partial^4 p(x,t)}{\partial x^4} \qquad (4\text{-}b)$$

Note that the fourth order term is negative in the governing equation. This assures stability with respect to small harmonic perturbations. Let us assume solutions of the type:

$$p(x,t) = \xi \exp\left(\omega t + \frac{x}{\lambda}i\right)$$

Introducing this expression in (4-b) we have:

$$\omega = -\frac{D\beta}{\lambda^2} - \rho\beta(1-\beta)\frac{1}{\lambda^4}$$

Since $0 \leq \beta \leq 1$, given that λ is real and both the diffusion and the retention coefficients are positive it follows that ω is always negative and the solution is stable for all wave length λ. Note that for positive fourth order term the solution may be unstable for small wave lengths. In this paper we will concentrate on the analysis of the solution of equation (4-b) and its dependence on the parameter β.

3. THE BOUNDARY CONDITIONS

Let us discuss the boundary conditions relative to the equation (4-a). The first two boundary conditions are classical. The first boundary condition is the concentration level at the boundary $x = \hat{x}$, that is:

$$p(\hat{x},t) = p_0(t) \qquad (5\text{-}a)$$

We will allow the boundary conditions to be functions time. The concentration gradient at the boundary gives the second boundary condition. This condition according to the Fick's law gives the flux $\phi_D(t)$ trough the boundary $x = \hat{x}$.

$$\left\|\vec{d}\right\| = -D\frac{\partial p(\hat{x},t)}{\partial x} = \phi_D(t)$$

or

$$D\frac{\partial p(\hat{x},t)}{\partial x} = -\frac{\phi_D(t)}{D} \qquad (5\text{-}b)$$

Now the third and the fourth boundary conditions are given by the second and the third derivatives of the function $p(x,t)$. The physical interpretation of these derivatives may be given by the following arguments. From the governing equation and assuming the continuity between the initial conditions and the boundary conditions to be sufficiently smooth it is possible to write:

$$\frac{\partial^2 p(\hat{x},t)}{\partial x^2} = \frac{1}{\beta D}\frac{\partial p(\hat{x},t)}{\partial t} + (1-\beta)\frac{\rho}{D}\frac{\partial^4 p(\hat{x},t)}{\partial x^4}$$

Now for most of the cases $\beta(1-\beta)\rho \ll 1$ from which follows:

$$\frac{\partial^2 p(\hat{x},t)}{\partial x^2} \approx \frac{1}{\beta D}\frac{\partial p(\hat{x},t)}{\partial t} \qquad (5\text{-}c)$$

Therefore the third boundary condition may be interpreted for most of the cases as proportional to the time variation of the concentration. The fourth boundary condition comes immediately from (5-c) by differentiation with respect to x:

$$\frac{\partial^3 p(\hat{x},t)}{\partial x^3} \approx \frac{1}{\beta D}\frac{\partial}{\partial x}\left(\frac{\partial p(\hat{x},t)}{\partial t}\right)$$

$$(5\text{-}d)$$

Then summarizing, for the classical one-dimensional problem, the boundary conditions regarding the value of the concentration function, and its first, second and third derivatives are related respectively with the following data specified at the boundary:

1. The concentration $p_0(t)$
2. The gradient of the concentration $grad(p_0(t))$
3. The time variation of the concentration $\partial p_0(t)/\partial t$
4. The gradient of the time variation of the concentration $grad(\partial p_0(t)/\partial t)$

Given the above values and the physical parameters the boundary conditions can be determined from the equations (5 a-d). More complex boundary conditions depend on the specificity of the problem under consideration. In any case they could be formulated using the appropriate combination of the foregoing conditions.

4. VARIATIONAL FORMULATION

Assuming that the region of interest is the domain $\Omega \subset R$ the weak solution associated to (eq. 4b) is the function $p(x)$ which satisfies:

$$\left(\frac{\partial p}{\partial t},\hat{p}\right)+\left(C_1\frac{\partial p}{\partial x},\frac{\partial \hat{p}}{\partial x}\right)+\left(C_2\frac{\partial^2 p}{\partial x^2},\frac{\partial^2 \hat{p}}{\partial x^2}\right)=0 \qquad \forall \hat{p} \in V$$

$$(u,w)=\int_\Omega u.w d\Omega; \qquad V \equiv H_0^2(\Omega)$$

$$C_1=\beta D; \quad C_2 = \beta(1-\beta)\rho$$

$H_0^2(\Omega)$ represents the classical Sobolev space of squared integrable functions with squared integrable first and second derivatives.
Remarks:

- Restriction of this form to a finite element subspace will lead to the well known Galerkin finite element method.

- The finite element subspace must be constructed such that the approximated solution and its first derivative be continuous at the nodal points. For 1-D problems these requirements are attained using Hermite's cubic interpolation.
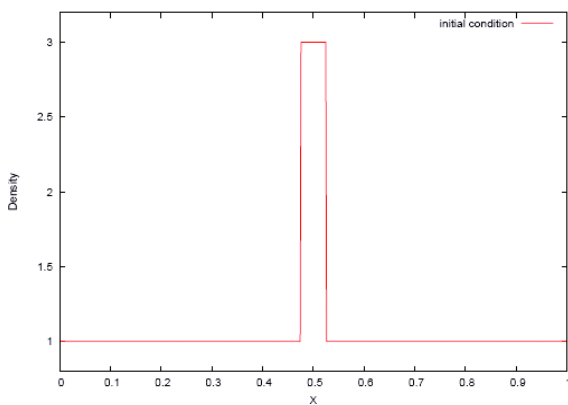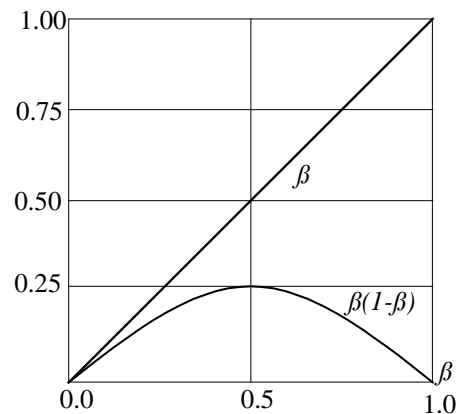

Fig.1 – Initial Condition

Fig.2 – The logistic curve β (1- β) for a linear variation of β

5. NUMERICAL EXPERIMENTS

In this section the numerical results of some performed experiments will be presented to highlight the influence of the parameter β on the diffusion-retention problem behavior. Those results were obtained using a semi-discrete version of the Galerkin method proposed in the preceding section. In each finite element Hermite's cubic interpolation is employed and a step-by-step procedure is adopted for the time evolution process. The domain of interest is the interval (0,1) and the boundary conditions were set as:

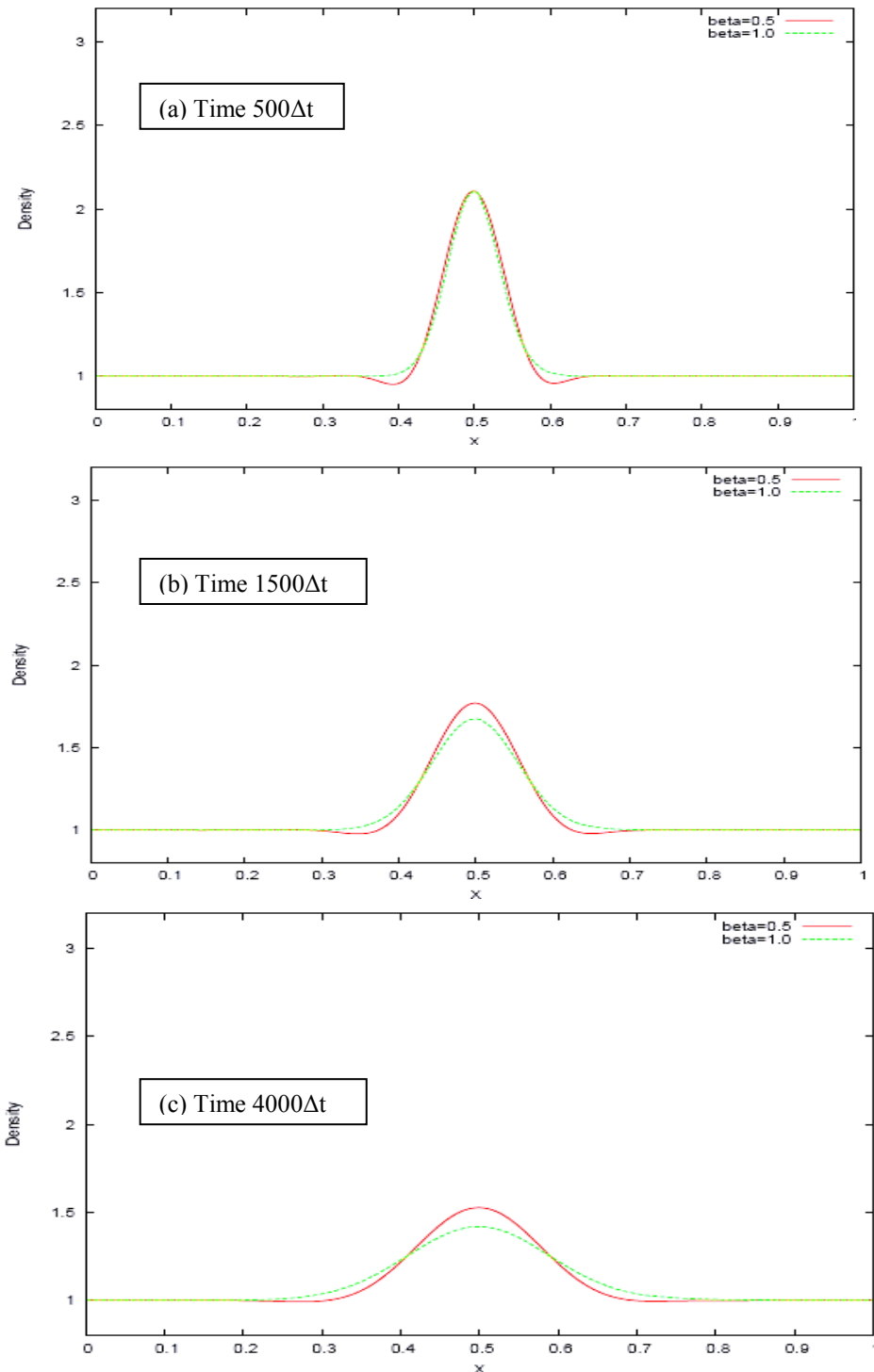$$p(0) = p(1) = 1; \quad C_2 \frac{\partial p}{\partial x}(0) = \frac{\partial p}{\partial x}(1) = 0$$

Fig.3 – Time history evolution of the population density distribution for β=0.5 and β=1
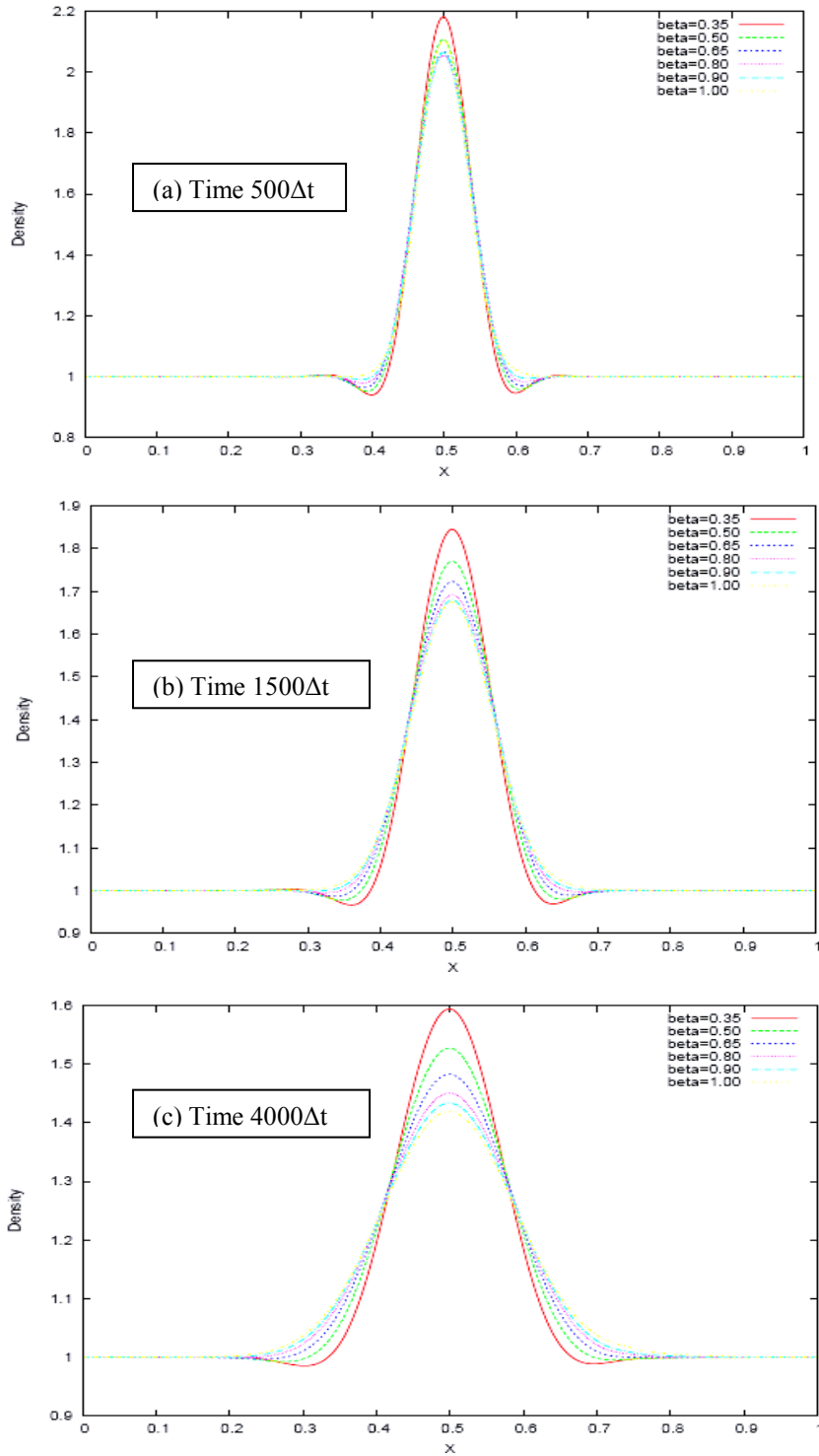
Fig.4 – Time history evolution of the population density distribution- 0.35,0.5,0.65,0.8,0.9)

The domain was discretized in 220 finite elements and a time-step of $\Delta t=10^{-3}$ was used. The diffusion coefficient was taken as $D=10^{-3}$ and the retention coefficient value was $\rho=10^{-6}$. The adopted initial condition is shown in figure 1, and to guide the choice of the value of the parameter β, it is depicted in figure 2 the relative weight of the diffusing and trapped particles in the process related with β and β (1- β) respectively. Notice that for $\beta=0.5$ the logistic curve reaches a maximum value of (0.25).

Figures (3a-c) and (4a-c) show the spatial distribution of the population density at times (500 Δt, 1500 Δt, 3000 Δt and 4000 Δt). In figures (3a-c) we compare the results for a purely diffusion process ($\beta=1.0$) and for the diffusion-retention process ($\beta=0.5$). From these results it becomes evident that the proposed model reproduces the expected behavior for diffusion-retention phenomena, in the sense that the added fourth order term diminishes the diffusion spreading velocity (see curves for $\beta=0.5$). Moreover, the appearance of the depression regions (values less than 1)

observed for the curves (β=0.5) agrees with the expected retention effects. In figures (4a-c) the calculated results for five different values of β (0.35, 0.5, 0.65, 0.8 and 0.9) are presented. These results are also in accordance with diffusion processes subjected to different amounts of retention Increasing β the retention effect reduces from a situation of total retention (β=0) to a purely diffusion phenomenon (β=1).

6. CONCLUSIONS

The solution to the problem of diffusion with retention was formulated for physic-chemical systems and the numerical simulations for the simple case of β constant provided encouraging results. The expected spreading delay induced by the retention process was clearly reproduced in the solutions. The diffusion-retention law proposed by the first time, as far as we know, introducing the fourth order term and the control parameter β, seems to simulate satisfactorily the physic-chemical phenomena provided that the supporting media and the particle system are homogeneous. Even for irregular media (Nicholson, Sykova,1998) the formulation may apply if the diffusion and retention coefficients are taken as average values.

Time delay for a different class of problem involving entropy distribution and fourth order partial differential equation matches closely the behavior produced by temporary retention as introduced here (Broadbridge P., 2008).

Despite experimental results are still missing the numerical simulation justify the investment in experimental research. We expect to start joint cooperation to design experimental arrangements to validate the theory. The introduction of a functional relation for the control parameter β depends very much on the experimental outcome.

7. ACKNOWLEDGEMENTS

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