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ANALYTICAL AND NUMERICAL STUDY OF MEMORY FORMALISMS IN DIFFUSION PROCESSES

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ABSTRACT: In this paper we study the diffusion of a liquid agent into a polymeric matrix. We propose a initial-boundary value problem to model the process. Numerical methods are obtained for solving it. The stability and the convergence of the methods are studied.

Key words: non-Fickian diffusion, viscoelastic behavior, drug delivery, finite difference methods,

Mathematics Subject Classification (2000): 65M06, 65M12, 65M15

1. Introduction

An important problem in controlled release technology is the diffusion of a penetrant into a polymeric carrier where a drug is dispersed. A suitable choice for simulating drug delivery can be the classical Fick's law. However to model the sorption of the liquid agent an equation that takes into account the viscoelastic nature of polymers and consequently its non Fickian behavior is needed ([6], [5], [8], [7], [11]). As the fluid penetrates the matrix, the polymeric structure changes, and the flux is not simply proportional to the concentration gradient. To obtain a more accurate description of the fluid penetration several modifications of the flux have been proposed in the literature by introducing a memory formalism ([6], [5]).

The main idea is that flux depends not only on the concentration gradient but also on the viscoelastic stress. In [6] the authors use a 3-parameter solid model [2] to describe the stress-strain relaxation. However the stability of the continuous model has not been studied. Also the authors do not develop specific numerical algorithms to discretize the non-Fickian model. When highly heterogeneous systems are considered [4] the memory formalism is introduced via factorial derivatives.

In this paper we study a non-Fickian diffusion mechanism described by a modified law for flux where diffusive and mechanical properties are coupled. We address the stability of the continuous problem and we develop numerical

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methods for which discrete energy estimates mimic the continuous ones. To take into account a wide range of mechanical behaviors we consider a general viscoelastic model [2] to describe the stress-strain relation. In particular the model in [5] can be obtained as a special case of the viscoelastic model studied here. Our results can be easily adapted to other mechanical models based on Maxwell generalized models [2]. We note that the class of models studied here can be used to simulate fluid flow in a porous media ([9], [10], [14]).

Let us recall that the Fickian diffusion of a penetrant is described by the conservation law

$$\frac{\partial C}{\partial t} = -div\ J_F\ , \tag{1}$$

where $C = C(t,x)$ is the fluid concentration and $J_F = J_F(t,x)$ represents the flux and is defined by

$$J_F(t,x) = -D\nabla C(t,x)\ , \tag{2}$$

where D is the diffusion coefficient for the penetrant fluid.

To take into account viscoelastic effects we consider a modified flux [3] expressed as the sum of a Fickian flux J_F and a non Fickian contribution J_{NF} defined by

$$J_{NF}(t,x) = -D_v\nabla\sigma(t,x)\ , \tag{3}$$

where $\sigma = \sigma(t,x)$ represents the stress and D_v stands for a stress-driven diffusion coefficient. The balance equation describing the behavior of the penetrant fluid is represented by

$$\frac{\partial C}{\partial t} = -div\ J\ , \tag{4}$$

where $J = J_F + J_{NF}$

In our model we assume that the change of volume due to the relaxation of the polymeric matrix is instantaneous [11]. Both D and D_v can depend in some cases on C, nevertheless, for analytical purposes these parameters can be considered to be positive constants. In fact although solvent diffusion coefficient depends on solvent concentration the hypothesis of a constant solvent diffusion can be accepted if the swelling process does not take place from a dry condition up to a swelling equilibrium, but takes place from a partially swollen condition to another one [12].

From (2), (3) and (4), we have

$$\frac{\partial C}{\partial t} = D\Delta C + D_v\Delta\sigma\ . \tag{5}$$

To model the viscoelastic polymeric behavior mechanical analog built with springs and dampers elements combined in a variety of arrangements are used [2]. We will consider a family of models, known as the 4-parameter solid model [2] that accounts for a wide range of viscoelastic behaviors. The arrangement is shown in Figure 1.

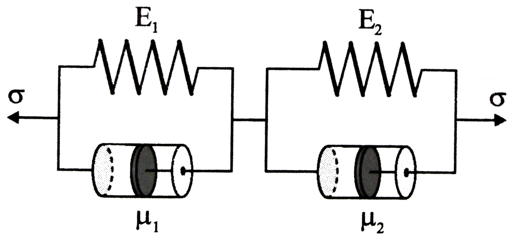

FIGURE 1. Four parameter solid model for viscoelastic polymeric behavior

The parameters E_1 and E_2 are non negative constants related with the elastic behavior of the polymer. The parameters μ_1 and μ_2 are also non negative constants related with the viscous behavior of the polymer (for more details see [2]). Note that different linear viscoelastic models can be obtained as a particular case of Figure 1.

For example taking $E_1 = \mu_2 = 0$, we obtain the Maxwell model. Let $\varepsilon(t,x)$ represent the strain. Assuming then that the strain and the concentration are proportional, that is, $\exists \alpha > 0$ such that $\varepsilon(t,x) = \alpha C(t,x)$, the family of models can be represented by the PDE [2]

$$\frac{\partial \sigma}{\partial t} + p_1 \sigma = q_0 C + q_1 \frac{\partial C}{\partial t} + q_2 \frac{\partial^2 C}{\partial t^2} \ , \tag{6}$$

where

$$p_1 = \frac{E_1 + E_2}{\mu_1 + \mu_2} \ , \ q_0 = \alpha \frac{E_1 E_2}{\mu_1 + \mu_2} \ , \ q_1 = \alpha \frac{E_2 \mu_1 + E_1 \mu_2}{\mu_1 + \mu_2} \quad and \quad q_2 = \alpha \frac{\mu_1 \mu_2}{\mu_1 + \mu_2} \ ,$$

The constants q_0, q_1, q_2 and p_1 have a physical meaning for the model and therefore they satisfy the following inequalities [2]

$$q_1^2 - 4 q_0 q_2 > 0 \quad and \quad q_1 p_1 - q_0 - q_2 p_1^2 > 0 \ . \tag{7}$$

2. The Model

We consider a polymer filling a bounded domain $\Omega \subset \mathbb{R}^n$ with boundary $\partial\Omega$. We study the diffusion of a penetrant in this polymer described by the following initial-boundary value problem:

$$\frac{\partial C}{\partial t} = D\Delta C + D_v \Delta\sigma \quad in \ \ (0,T] \times \Omega \ , \tag{8}$$

$$\frac{\partial \sigma}{\partial t} + p_1\sigma = q_o C + q_1 \frac{\partial C}{\partial t} + q_2 \frac{\partial^2 C}{\partial t^2} \quad in \ \ (0,T] \times \Omega \ , \tag{9}$$

$$C(t,x) = C_b, \quad \sigma(t,x) = \sigma_b, \quad (t,x) \in (0,T] \times \partial\Omega \ , \tag{10}$$

$$C(0,x) = C_0(x), \quad \sigma(0,x) = \sigma_0, \quad x \in \Omega \ . \tag{11}$$

Here $C : [0,T] \times \bar{\Omega} \to \mathbb{R}$ is the unknown concentration of the penetrant, $\sigma : [0,T] \times \bar{\Omega} \to \mathbb{R}$ is the unknown stress, $C_0 : \bar{\Omega} \to \mathbb{R}$ is the given initial concentration of the liquid in the matrix, $\sigma_0 \in \mathbb{R}$ is the given initial stress in the matrix, $C_b \in \mathbb{R}$ is the given concentration of the liquid in the fully swollen matrix, $\sigma_b \in \mathbb{R}$ is the given stress in the fully swollen gel. We observe that Ω is fixed in time because the change of volume due to swelling is supposed to occur instantaneously.

3. Energy estimates for the continuous problem

By $C(t)$ we represent a function defined from $\bar{\Omega}$ into $\mathbb{R}^2$ with t fixed. Using energy estimates techniques we study in this section the stability of model (8)-(11).

We begin by integrating equation (9) over time to obtain

$$\begin{aligned} \sigma(t) &= (q_2p_1 - q_1)C_0 e^{-p_1 t} + (q_1 - q_2p_1)C(t) \\ &\quad +(q_0 + q_2p_1^2 - q_1p_1)\int_0^t e^{p_1(s-t)}C(s)ds + q_2\frac{\partial C}{\partial t}(t) + e^{-p_1 t}\sigma_0 \ . \end{aligned}$$

Replacing this last equation in (8) and rearranging the terms, we have

$$\frac{\partial C}{\partial t}(t) = A\Delta\frac{\partial C}{\partial t}(t) + B\Delta C(t) + F\int_0^t e^{p_1(s-t)}\Delta C(s)ds + Ge^{-p_1 t}\Delta C_0 \ , \tag{12}$$

where

$$A = D_v q_2, \ B = D + D_v(q_1 - q_2p_1), \ F = D_v(q_0 + q_2p_1^2 - q_1p_1) \tag{13}$$

and

$$G = D_v(q_2p_1 - q_1) \ .$$

We note that from (7) we can conclude that $A, B > 0$ and $F, G < 0$.

As we are interested in studying the stability of (8)-(11) we assume without loss of generality that

$$C(t,x)=0, \quad (t,x)\in [0,T]\times \partial\Omega \ . \tag{14}$$

The initial-boundary value problem (11), (12), (14), with $A=0$, is a special case of the general parabolic integro-differential problem

$$u_t=\nabla.\left\{a(u)\nabla u+\int_0^t b(s)\nabla u(s)ds\right\}+f(u) \quad in \ (0,T]\times\Omega \ , \tag{15}$$

$$u(t,x)=0, \quad (t,x)\in (0,T]\times\partial\Omega \ , \tag{16}$$

$$u(0,x)=u_0(x), \quad x\in\Omega \ , \tag{17}$$

where a,b and f are known functions. Problem (15)-(17) can serve as a model of fluid flow in porous media problems, specially in physical processes where significant memory effects can occur. For the details of formulation and their physical interpretations we refer the reader to ([9], [10], [14], [15]).

Let $(.,.)$ denote the inner product in $L^2(\Omega)$ and $\|.\|_2$ the usual norm induced by $(.,.)$. Let $H_0^1(\Omega)$ be the usual Sobolev space. By $W^{1,\infty}(0,T;H_0^1(\Omega))$ we represent the space of functions $v: \ (0,T)\mapsto H_0^1(\Omega)$ such that

$$\sum_{i=1}^n \underset{[0,T]}{ess \ sup}\left\|\frac{d^iv}{dt^i}\right\|_{H^1}<\infty \ .$$

By $|.|_{H^1}$ we represent the usual seminorm in $H_0^1(\Omega)$. We replace (11), (12), (14) by the following variational problem: find $C\in W^{1,\infty}(0,T;H_0^1(\Omega))$ such that

$$(\frac{dC}{dt}(t),v)+A(\nabla\frac{dC}{dt}(t),\nabla v)+B(\nabla C(t),\nabla v)+F(\int_0^t e^{p_1(s-t)}\nabla C(s)ds,\nabla v)$$
$$=G(e^{-p_1t}\Delta C_0,v) \qquad a.e \ in \ (0,T), \ \ \forall \ v\in H_0^1(\Omega) \ , \tag{18}$$

and

$$C(0)=C_0 \ , \tag{19}$$

where

$$(\nabla u,\nabla v)=\sum_{i=1}^n(\frac{\partial u}{\partial x_i},\frac{\partial v}{\partial x_i}), \quad u,v\in H_0^1(\Omega) \ .$$

We establish in what follows an estimate for the energy functional

$$\mathbb{E}(C)(t)=\|C(t)\|_2^2+A\,|C(t)|_{H^1}^2+2B\int_0^t|C(s)|_{H^1}^2\,ds \ , \tag{20}$$

where A and B are defined in (13).

Theorem 1. *Let C be a solution of (18), (19) in $W^{1,\infty}(0,T;H_0^1(\Omega))$, then*

$$\mathbb{E}(C)(t) \leq \left(\|C_0\|_2^2 + A\,|C_0|_{H^1}^2 + \frac{3\,|G|^2}{2p_1 A\phi}\,|C_0|_{H^1}^2 \right) e^{t\phi}\ , \tag{21}$$

where $\phi = \sqrt{\frac{3|F|^2}{8BAp_1}}$.

Proof: Considering in (18) $v = C(t)$ we easily deduce

$$\begin{aligned} &\frac{d}{dt}\,\|C(t)\|_2^2 + A\frac{d}{dt}\,|C(t)|_{H^1}^2 + 2B\,|C(t)|_{H^1}^2 \\ &\ = \ 2\,|F| \int_0^t e^{p_1(s-t)}(\nabla C(s), \nabla C(t))ds + 2\,|G|\,e^{-p_1 t}(\nabla C_0, \nabla C(t))\ . \end{aligned} \tag{22}$$

Let us estimate the two terms in the second member of (22). We have

$$\begin{aligned} 2\,|F| \int_0^t e^{p_1(s-t)}\,|(\nabla C(s), \nabla C(t))|\,ds \ &\leq\ 2\,|F| \int_0^t e^{p_1(s-t)}\,|C(s)|_{H^1}\,|C(t)|_{H^1}\,ds \\ &\leq\ 2\epsilon\,|C(t)|_{H^1}^2 \\ &\quad + \frac{|F|^2}{2\epsilon}\left(\int_0^t e^{p_1(s-t)}\,|C(s)|_{H^1}\,ds \right)^2 \\ &\leq\ 2\epsilon\,|C(t)|_{H^1}^2 + \frac{|F|^2}{2\epsilon}\psi \left(\int_0^t |C(s)|_{H^1}^2\,ds \right)\ , \end{aligned}$$

where $\epsilon > 0$ is an arbitrary constant and ψ satisfies

$$\psi = \int_0^t e^{2p_1(s-t)}ds \leq \frac{1}{2p_1}\ .$$

As we also have that

$$2\,|G|\,e^{-p_1 t}(\nabla C_0, \nabla C(t)) \leq \frac{|G|^2\,e^{-2p_1 t}}{\epsilon}\,|C_0|_{H^1}^2 + \epsilon\,|C(t)|_{H^1}^2\ ,$$

we can establish from (22) that

$$\frac{d}{dt}\left(\|C(t)\|_2^2 + A\,|C(t)|_{H^1}^2 + 2B\int_0^t |C(s)|_{H^1}^2\,ds\right)$$
$$\leq\; 3\epsilon\,|C(t)|_{H^1}^2 + \frac{|F|^2}{4p_1\epsilon}\left(\int_0^t |C(s)|_{H^1}^2\,ds\right) + \frac{|G|^2\,e^{-2p_1 t}}{\epsilon}\,|C_0|_{H^1}^2\;\;.$$

Adding the term $\frac{3\epsilon}{A}\|C(t)\|_2^2$ to the right hand side, integrating and rearranging the terms we get

$$\|C(t)\|_2^2 + A\,|C(t)|_{H^1}^2 + 2B\int_0^t |C(s)|_{H^1}^2\,ds$$
$$\leq\; \int_0^t \frac{3\epsilon}{A}\left(\|C(s)\|_2^2 + A\,|C(s)|_{H^1}^2 + \frac{|F|^2 A}{12p_1\epsilon^2}\int_0^s |C(r)|_{H^1}^2\,dr\right)ds$$
$$+\,\|C_0\|_2^2 + A\,|C_0|_{H^1}^2 + \frac{|G|^2}{2p_1\epsilon}\,|C_0|_{H^1}^2\;\;.$$

Since ϵ is an arbitrary constant, we take $\epsilon = \sqrt{\frac{|F|^2 A}{24Bp_1}}$. Then we finally conclude

$$\mathbb{E}(C)(t) \leq \|C_0\|_2^2 + A\,|C_0|_{H^1}^2 + \frac{|G|^2}{2p_1\epsilon}\,|C_0|_{H^1}^2 + \int_0^t \phi\mathbb{E}(C)(s)ds\;,$$

where $\phi = \sqrt{\frac{3|F|^2}{8BAp_1}}$, and by the Gronwall Lemma [13], equation (21) holds. ■

We note that under the assumptions of Theorem 1, if (18), (19) has a solution C in $W^{1,\infty}(0,T;H_0^1(\Omega))$, then C is unique. In fact let C and $\hat{C}$ be two different solutions of (18), (19) such that both of them are in $W^{1,\infty}(0,T;H_0^1(\Omega))$, then $w = C - \hat{C} \in W^{1,\infty}(0,T;H_0^1(\Omega))$ is a solution of (18) with homogeneous initial condition. By Theorem 1 we conclude that

$$\mathbb{E}(w)(t) = 0\;,$$

consequently

$$C = \hat{C}\;,\quad \nabla C = \nabla\hat{C}\;\; in\;L^2(\Omega)\;.$$

In what follows we consider the stability behavior of C under perturbations in the initial condition C_0. Let C and $\hat{C}$ be solutions of (18), (19) in $W^{1,\infty}(0,T;H_0^1(\Omega))$ with initial conditions C_0 and $\hat{C}_0$ respectively. Then $w = C - \hat{C} \in W^{1,\infty}(0,T;H_0^1(\Omega))$ satisfies (18) with $w = 0$ in $(0,T]\times\partial\Omega$ and

$w(0) = C_0 - \hat{C}_0$ in Ω. Consequently from the proof of Theorem 1 it follows that

$$\mathbb{E}(w)(t) \leq \left(\left\| C_0 - \hat{C}_0 \right\|_2^2 + A \left| C_0 - \hat{C}_0 \right|_{H^1}^2 + \frac{3\,|G|^2}{2p_1 A\phi} \left| C_0 - \hat{C}_0 \right|_{H^1}^2 \right) e^{t\phi} \ ,$$

which implies that (18), (19) is stable in bounded time intervals.

4. Energy estimates for the semi-discrete approximation

The semi-discrete problem is studied for $n = 1$ and $\Omega = [a, b]$. Let us consider in $[a, b]$ a grid $I_h = \{x_i,\ i = 0, 1, .., N\}$ with $x_0 = a$, $x_N = b$ and $x_i - x_{i-1} = h$. Let u_h be a function defined over I_h and $L^2(I_h)$ the space of grid functions defined in I_h. For $u_h \in L^2(I_h)$ we introduce the following finite-difference operators

$$\begin{aligned} D_{-x}u_h(x_i) &= \frac{u_h(x_i) - u_h(x_{i-1})}{h} \ , \\ D_{2,x}u_h(x_i) &= \frac{u_h(x_{i+1}) - 2u_h(x_i) + u_h(x_{i-1})}{h^2} \ . \end{aligned}$$

By $L^2_0(I_h)$ we represent the subspace of $L^2(I_h)$ of functions null on the boundary points. For grid functions u_h and v_h in $L^2_0(I_h)$ we introduce the inner product

$$(u_h, v_h)_h = \sum_{i=1}^{N-1} h u_h(x_i) v_h(x_i) \ .$$

We denote by $\|.\|_h$ the norm induced by the above inner product. For grid functions u_h and v_h in $L^2(I_h)$ we introduce the notations

$$(u_h, v_h)_+ = \sum_{i=1}^{N} h u_h(x_i) v_h(x_i) \ ,$$

and

$$\|u_h\|_+^2 = \sum_{i=1}^{N} h (u_h(x_i))^2 \ ,$$

Discretizing the partial spatial derivative that arise in (18) we introduce the semi-discrete approximation $C_h(t)$ for the solution C of (18), (19). The semi-discrete variational problem has the form

$$
\begin{aligned}
&(\frac{dC_h}{dt}(t), v_h)_h + A(D_{-x}\frac{dC_h}{dt}(t), D_{-x}v_h)_+ + B(D_{-x}C_h(t), D_{-x}v_h)_+ \\
&+F(\int_0^t e^{p_1(s-t)} D_{-x}C_h(s)ds, D_{-x}v_h)_+ = G(e^{-p_1 t}D_{2,x}C_0, v_h)_h \\
&a.e\ in\ (0,T]\ \ \forall\ v_h \in L_0^2(I_h),
\end{aligned} \tag{23}
$$

and

$$
C_h(0) = R_h C_0\ , \tag{24}
$$

where $R_h : \mathcal{C}([a,b]) \mapsto \mathbb{R}$ denote the pointwise restriction operator

$$
R_h u(x_i) = u(x_i)\ \ for\ \ i = 1,2,..,N\ .
$$

It can be shown that if $C_h \in \mathcal{C}^1(0,T; L_0^2(I_h))$ which denotes the space of functions $u_h : [0,T] \mapsto L_0^2(I_h)$ which have first time continuous derivative with respect to the norm $\|.\|_h$, then C_h is solution of the following ordinary differential problem

$$
\begin{aligned}
\frac{dC_h}{dt}(t) &= AD_{2,x}\frac{dC_h}{dt}(t) + BD_{2,x}C_h(t) + F\int_0^t e^{p_1(s-t)} D_{2,x}C_h(s)ds \\
&\quad +Ge^{-p_1 t}D_{2,x}C_h(0)\ ,
\end{aligned} \tag{25}
$$

for $t \in (0,T]$,

$$
C_h(t,x_0) = C_h(t,x_N) = 0,\ for\ all\ t \in [0,T]\ , \tag{26}
$$

$$
C_h(0,x_i) = C_0(x_i),\ for\ \ i = 1,2,...,N-1\ . \tag{27}
$$

In what follows we establish an estimate for a semi-discrete version of (20),

$$
\mathbb{E}(C_h)(t) = \|C_h(t)\|_h^2 + A\|D_{-x}C_h(t)\|_+^2 + 2B\int_0^t \|D_{-x}C_h(s)\|_+^2\, ds\ .
$$

Theorem 2. *Let C_h be a solution of (23), (24), then*

$$
\mathbb{E}(C_h)(t) \le \left(\|C_h(0)\|_h^2 + A\|D_{-x}C_h(0)\|_+^2 + \frac{3|G|^2}{2p_1 A\phi}\|D_{-x}C_h(0)\|_+^2 \right) e^{t\phi}\ , \tag{28}
$$

where $\phi = \sqrt{\frac{3|F|^2}{8BAp_1}}$.

Proof: Let C_h be a solution of (23), (24). Then considering $v_h = C_h(t)$ we have

$$\begin{aligned} \frac{d}{dt}\left(\|C_h(t)\|_h^2 + A\,\|D_{-x}C_h(t)\|_+^2 + 2B\int_0^t \|D_{-x}C_h(s)\|_+^2\,ds\right) \\ = \; 2\,|F|\int_0^t e^{p_1(s-t)}\left(D_{-x}C_h(s), D_{-x}C_h(t)\right)_+ ds \\ +2\,|G|\,e^{-p_1 t}\left(D_{-x}C_0, D_{-x}C_h(t)\right)_+ \;. \end{aligned} \tag{29}$$

As

$$\begin{aligned} & 2\,|F|\int_0^t e^{p_1(s-t)}\left(D_{-x}C_h(s), D_{-x}C_h(t)\right)_+ ds \\ & \le \; 2\epsilon\,\|D_{-x}C_h\|_+^2 + \frac{|F|^2}{2\epsilon}\left(\int_0^t e^{2p_1(s-t)}ds\right)\int_0^t \|D_{-x}C_h(s)\|_+^2\,ds \;, \end{aligned}$$

and

$$\begin{aligned} 2\,|G|\,e^{-p_1 t}\sum_{i=1}^N h\,|D_{-x}C_0(x_i)D_{-x}C_h(t,x_i)| \; & \le \; \frac{|G|^2\,e^{-2p_1 t}}{\epsilon}\,\|D_{-x}C_0(x)\|_+^2 \\ & +\epsilon\,\|D_{-x}C(t,x)\|_+^2 \;, \end{aligned}$$

where $\epsilon > 0$ is an arbitrary constant, we have from (29)

$$\begin{aligned} \frac{d}{dt}\mathbb{E}(C_h(t)) \; & \le \; 3\epsilon\,\|D_{-x}C_h(t)\|_+^2 + \frac{|F|^2}{4p_1\epsilon}\int_0^t \|D_{-x}C_h(s)\|_+^2\,ds \\ & + \frac{|G|^2\,e^{-2p_1 t}}{\epsilon}\,\|D_{-x}C_h(0)\|_+^2 . \end{aligned}$$

Following the proof of Theorem 1, we conclude (28). ■

Analogously as in the continuous case we consider the stability behavior of C_h under perturbations in the initial condition $C_h(0)$. Let C_h and $\hat{C}_h$ be solutions of (23), (24) with initial conditions $C_h(0)$ and $\hat{C}_h(0)$ respectively. Then $w_h = C_h - \hat{C}_h$ satisfies (23) with $w_h(0) = C_h(0) - \hat{C}_h(0)$ in $[a, b]$.

Consequently from the proof of Theorem 2 it follows that

$$\begin{aligned}\mathbb{E}(w_h)(t) \ \leq \ & \left(\left\|C_h(0)-\hat{C}_h(0)\right\|_h^2 + A\left\|D_{-x}(C_h(0)-\hat{C}_h(0))\right\|_+^2\right.\\ & \left. +\frac{3\,|G|^2}{2p_1 A\phi}\left\|D_{-x}(C_h(0)-\hat{C}_h(0))\right\|_+^2\right) e^{t\phi}\ , \qquad (30)\end{aligned}$$

which implies that (23), (24) is stable in bounded time intervals.

5. Error estimates for the semi-discrete approximation

By $E_h(t)$ we represent the error induced by the spatial discretization introduced before. $E_h(t) = R_hC(t) - C_h(t)$ where $C_h(t)$ is the solution of (23)-(24).

In the convergence analysis we assume that the solution of (11), (12), (14), C belongs to the space $W^{1,\infty}(0,T;H_0^3(a,b))$ which is defined as $W^{1,\infty}(0,T;H_0^1(a,b))$ replacing $H_0^1(a,b)$ by $H_0^3(a,b)$.

Theorem 3. *Let C and C_h be the solutions of (18), (19) and (23), (24), respectively. If $C \in W^{1,\infty}(0,T;H_0^3(a,b))$, then*

$$\mathbb{E}(E_h(t)) \leq e^{\phi t}\left(\|E_h(0)\|_h^2 + A\,\|D_{-x}E_h(0)\|_+^2\right) + h^4\int_0^t K(z)e^{\phi(t-z)}dz\ , \qquad (31)$$

where

$$\begin{aligned}K(t) \ = \ & \frac{20\beta_1^2}{\phi A}\left[A^2\left|\frac{\partial C}{\partial t}(t)\right|_{H^3}^2 + B^2\,|C(t)|_{H^3}^2 + F^2\int_0^t e^{p_1(s-t)}\,|C(s)|_{H^3}^2\,ds\right.\\ & \left. +G^2\,|C_0|_{H^3}^2\right] + \frac{4\beta_2^2}{\phi}\left|\frac{\partial C}{\partial t}(t)\right|_{H^2}^2\ .\end{aligned}$$

with ϕ, β_1 and β_2 positive constants.

Proof: As we have

$$\begin{aligned}\frac{dE_h}{dt}(t) \ = \ & R_h\frac{\partial C(t)}{\partial t}(t) - \left[AD_{2,x}\frac{dC_h}{dt}(t) + BD_{2,x}C_h(t)\right.\\ & \left. +F\int_0^t e^{p_1(s-t)}D_{2,x}C_h(s)ds + Ge^{-p_1 t}D_{2,x}C_0\right]\ ,\end{aligned}$$

we easily deduce that

$$\begin{aligned}(\frac{dE_h}{dt}(t), E_h(t))_h &= (R_h\frac{\partial C}{\partial t}(t), E_h(t))_h + A(D_{-x}\frac{dC_h}{dt}(t), D_{-x}E_h(t))_+ \\ &\quad + B(D_{-x}C_h(t), D_{-x}E_h(t))_+ \\ &\quad + F\int_0^t e^{p_1(s-t)}(D_{-x}C_h(s), D_{-x}E_h(t))_+ ds \\ &\quad + Ge^{-p_1 t}(D_{-x}C_0, D_{-x}E_h(t))_+ \ . \end{aligned} \tag{32}$$

Let $\left(\hat{\frac{\partial C}{\partial t}}\right)_h(t)$ be the following grid function

$$\left(\hat{\frac{\partial C}{\partial t}}\right)_h(t, x_i) = \frac{1}{h}\int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}} \frac{\partial C}{\partial t}(t)dx \ ,$$

where $x_{\frac{i-1}{2}} = \frac{x_{i-1}+x_i}{2}$ and $x_{\frac{i+1}{2}} = \frac{x_i+x_{i+1}}{2}$, for $i = 1, 2, .., N-1$.

Introducing $\left(\hat{\frac{\partial C}{\partial t}}\right)_h(t)$ in (32) we deduce

$$\begin{aligned}(\frac{dE_h}{dt}(t), E_h(t))_h &= (R_h\frac{\partial C}{\partial t}(t) - \left(\hat{\frac{\partial C}{\partial t}}\right)_h(t), E_h(t))_h + (\left(\hat{\frac{\partial C}{\partial t}}\right)_h(t), E_h(t))_h \\ &\quad + A(D_{-x}\frac{dC_h}{dt}(t), D_{-x}E_h(t))_+ + B(D_{-x}C_h(t), D_{-x}E_h(t))_+ \\ &\quad + F\int_0^t e^{p_1(s-t)}(D_{-x}C_h(s), D_{-x}E_h(t))_+ ds \\ &\quad + Ge^{-p_1 t}(D_{-x}C_0, D_{-x}E_h(t))_+ \ . \end{aligned} \tag{33}$$

We remark that

$$\begin{aligned}(\left(\hat{\frac{\partial C}{\partial t}}\right)_h(t), E_h(t))_h &= \sum_{i=1}^{N-1} h\int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}} \frac{\partial C}{\partial t}(t)dx E_h(t, x_i) \\ &= \sum_{i=1}^{N-1} h\int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}} \left(A\frac{\partial^2}{\partial x^2}\left(\frac{\partial C}{\partial t}\right)(t) + B\frac{\partial^2 C}{\partial x^2}(t)\right. \\ &\quad \left. + F\int_0^t e^{p_1(s-t)}\frac{\partial^2 C}{\partial x^2}(s)ds + Ge^{-p_1 t}\frac{\partial^2 C_0}{\partial x^2}\right) dx E_h(t, x_i) \ . \end{aligned} \tag{34}$$

Using summation by parts it is easy to see that

$$\sum_{i=1}^{N-1}\left(\int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}}\frac{\partial^2 g}{\partial x^2}(x)dx\right)E_h(t,x_i) = -\sum_{i=1}^{N} h\frac{\partial g}{\partial x}(x_{\frac{i-1}{2}})D_{-x}E_h(t,x_i)\ . \quad (35)$$

Let $\hat{R}_h$ be defined by $\hat{R}_h g(x_i) = g(x_{\frac{i-1}{2}})$. Applying (35) to each term of (34) we easily establish the following

$$\begin{aligned}
(\left(\frac{\partial \hat{C}}{\partial t}\right)_h(t), E_h(t))_h \;=\; & -A(\hat{R}_h\left(\frac{\partial^2 C}{\partial x \partial t}\right)(t), D_{-x}E_h(t))_+ \\
& -B(\hat{R}_h\left(\frac{\partial C}{\partial x}\right)(t), D_{-x}E_h(t))_+ \\
& -F\int_0^t e^{p_1(s-t)}(\hat{R}_h\left(\frac{\partial C}{\partial x}\right)(s), D_{-x}E_h(t))_+ ds \\
& -Ge^{-p_1 t}(\hat{R}_h\left(\frac{\partial C_0}{\partial x}\right), D_{-x}E_h(t))_+ \\
=\; & A(D_{-x}R_h\left(\frac{\partial C}{\partial t}\right)(t) - \hat{R}_h\left(\frac{\partial^2 C}{\partial x \partial t}\right)(t), D_{-x}E_h(t))_+ \\
& +B(D_{-x}R_hC(t) - \hat{R}_h\left(\frac{\partial C}{\partial x}\right)(t), D_{-x}E_h(t))_+ \\
& +F\int_0^t e^{p_1(s-t)}(D_{-x}R_hC(s) \\
& -\hat{R}_h\left(\frac{\partial C}{\partial x}\right)(s), D_{-x}E_h(t))_+ ds \\
& -Ge^{-p_1 t}(\hat{R}_h\left(\frac{\partial C_0}{\partial x}\right), D_{-x}E_h(t))_+ \\
& -A(D_{-x}R_h\left(\frac{\partial C}{\partial t}\right)(t), D_{-x}E_h(t))_+ \\
& -B(D_{-x}R_hC(t), D_{-x}E_h(t))_+ \\
& -F\int_0^t e^{p_1(s-t)}(D_{-x}R_hC(s), D_{-x}E_h(t))_+ ds\ . \quad (36)
\end{aligned}$$

From (33) and from (36) we obtain

$$
\begin{aligned}
(\frac{dE_h}{dt}(t), E_h(t))_h &= -A(D_{-x}\frac{dE_h}{dt}(t), D_{-x}E_h(t))_+ - B(D_{-x}E_h(t), D_{-x}E_h(t))_+ \\
&\quad + |F| \int_0^t e^{p_1(s-t)}(D_{-x}E_h(s), D_{-x}E_h(t))_+ ds + T \ , \qquad (37)
\end{aligned}
$$

where $T = T_1 + T_2 + T_3 + T_4 + T_5$, with

$$
\begin{aligned}
T_1 &= (R_h \frac{\partial C(t)}{\partial t} - \left(\frac{\partial \hat{C}}{\partial t}\right)_h (t), E_h(t))_h \ , \\
T_2 &= A(D_{-x}R_h\left(\frac{\partial C}{\partial t}\right)(t) - \hat{R}_h\left(\frac{\partial^2 C}{\partial x \partial t}\right)(t), D_{-x}E_h(t))_+, \\
T_3 &= B(D_{-x}R_h C(t) - \hat{R}_h\left(\frac{\partial C}{\partial x}\right)(t), D_{-x}E_h(t))_+ \ , \\
T_4 &= F\int_0^t e^{p_1(s-t)}(D_{-x}R_h C(s) - \hat{R}_h\left(\frac{\partial C}{\partial x}\right)(s), D_{-x}E_h(t))_+ ds \ , \\
T_5 &= Ge^{-p_1 t}(D_{-x}C_0 - \hat{R}_h\left(\frac{\partial C_0}{\partial x}\right), D_{-x}E_h(t))_+ \ .
\end{aligned}
$$

As

$$
\begin{aligned}
& 2\,|F| \int_0^t e^{p_1(s-t)}(D_{-x}E_h(s), D_{-x}E_h(t))_+ ds \\
& \leq 2\epsilon \left\|D_{-x}E_h(t)\right\|_+^2 + \tfrac{|F|^2}{4p_1\epsilon}\int_0^t \left\|D_{-x}E_h(s)\right\|_+^2 ds \ ,
\end{aligned}
$$

where ϵ is an arbitrary positive constant, then by (37)

$$
\begin{aligned}
& \frac{d}{dt}\left(\left\|E_h(t)\right\|_h^2 + A\left\|D_{-x}E_h(t)\right\|_+^2 + 2B\int_0^t \left\|D_{-x}E_h(s)\right\|_+^2 ds\right) \\
& \leq 2\epsilon \left\|D_{-x}E_h(t)\right\|_+^2 + \tfrac{|F|^2}{4p_1\epsilon}\int_0^t \left\|D_{-x}E_h(s)\right\|_+^2 ds + 2\,|T| \ . \qquad (38)
\end{aligned}
$$

To estimate $T_2,\ T_3,\ T_4$ and T_5 we observe that

$$
\lambda(g) = D_{-x}g(x_i) - g(x_{\frac{i-1}{2}}) = \frac{1}{h}\left[V(0) - V(1) + V'(\frac{1}{2})\right] \ ,
$$

with $V(\xi) = g(x_i - h\xi)$.

Let $\lambda(V) = V(0) - V(1) + V'(\frac{1}{2})$. As we have

$$
\lambda(1) = 0, \quad \lambda(\xi) = 0, \quad \lambda(\xi^2) = 0 \ \ and \ \ \lambda(\xi^3) \neq 0 \ ,
$$

by the Bramble-Hilbert lemma [1] we deduce

$$|\lambda(v)| \leq \beta \int_0^1 \left|V^{'''}(\xi)\right| d\xi = h^2\beta \int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}} \left|g^{'''}(x)\right| dx \ ,$$

then

$$\begin{aligned} &\left|\sum_{i=1}^N h\left(D_{-x}g(x_i) - g(x_{\frac{i-1}{2}})\right) D_{-x}E_h(t,x_i)\right| \\ &\leq \ \beta \sum_{i=1}^N h^2 \int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}} \left|g^{'''}(x)\right| dx \, |D_{-x}E_h(t,x_i)| \\ &\leq \ \beta \sum_{i=1}^N h^2 \left(\int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}} \left|g^{'''}(x)\right|^2 dx\right)^{\frac{1}{2}} \sqrt{h}\, |D_{-x}E_h(t,x_i)| \\ &\leq \ \frac{\beta^2 h^4}{\epsilon} \sum_{i=1}^N |g|^2_{H^3\left[x_{\frac{i-1}{2}}, x_{\frac{i+1}{2}}\right]} + \epsilon \left\|D_{-x}E_h(t)\right\|_+^2 \ , \end{aligned}$$

that is

$$\left|\sum_{i=1}^N h\left(D_{-x}g(x_i) - g(x_{\frac{i-1}{2}})\right) D_{-x}E_h(t,x_i)\right| \leq \frac{\beta^2 h^4}{\epsilon} |g|^2_{H^3} + \epsilon \left\|D_{-x}E_h(t)\right\|_+^2 \ . \tag{39}$$

Considering (39) for $T_2,\ T_3,\ T_4$ and T_5 we obtain

$$\begin{aligned} \sum_{i=2}^5 |T_i| \ \leq \ & \frac{\beta_1^2}{\epsilon} h^4 \left[A^2 \left|\frac{\partial C}{\partial t}(t)\right|^2_{H^3} + B^2 |C(t)|^2_{H^3} + G^2 |C_0|^2_{H^3}\right. \\ & \left. + F^2 \int_0^t e^{p_1(s-t)} |C(s)|^2_{H^3} ds\right] + 4\epsilon \left\|D_{-x}E_h(t)\right\|_+^2 \ , \end{aligned} \tag{40}$$

for certain positive constant β_1.

To estimate T_1 we introduce now $l(g)$ defined by

$$\begin{aligned} l(g) &= hg(x_i) - \int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}} g(x)dx \\ &= hg(x_i) - h\int_0^1 g(x_{\frac{i-1}{2}} + h\xi)d\xi \\ &= h(V(\frac{1}{2}) - \int_0^1 V(\xi)d\xi) \ , \end{aligned}$$

with $V(\xi) = g(x_{\frac{i-1}{2}} + h\xi)$.

For $\lambda(V) = V(\frac{1}{2}) - \int_0^1 V(\xi)d\xi$ holds the following

$$\lambda(1) = 0, \quad \lambda(\xi) = 0, \quad and \quad \lambda(\xi^2) \neq 0 \ ,$$

then by the Bramble-Hilbert lemma [1] we obtain

$$|\lambda(V)| \leq \beta_2 \int_0^1 \left| V^{''}(\xi) \right| d\xi = h\beta_2 \int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}} \left| g^{''}(x) \right| dx \ ,$$

consequently we deduce for T_1

$$\begin{aligned} |T_1| &\leq \left| \beta_2 \sum_{i=1}^N h^2 \int_{x_{\frac{i-1}{2}}}^{x_{\frac{i+1}{2}}} \frac{\partial^3 C}{\partial^2 x \partial t}(x)dx E_h(t,x_i) \right| \\ &\leq \frac{\beta_2^2 A}{5\epsilon} h^4 \left| \frac{\partial C}{\partial t}(t) \right|_{H^2}^2 + \frac{5\epsilon}{A} \|E_h(t)\|_+^2 \ . \end{aligned} \tag{41}$$

Replacing (40) and (41) in (38) we obtain

$$\begin{aligned} \frac{d}{dt}\left(\mathbb{E}(E_h(t))\right) &\leq \frac{10\epsilon}{A} \|E_h(t)\|_h^2 + 10\epsilon \|D_{-x}E_h(t)\|_+^2 \\ &\quad + \frac{|F|^2}{4p_1\epsilon} \int_0^t \|D_{-x}E_h(s)\|_+^2 ds + h^4 K(t) \ , \end{aligned} \tag{42}$$

where

$$\begin{aligned} K(t) &= \frac{2\beta_1^2}{\epsilon} \left[A^2 \left| \frac{\partial C}{\partial t}(t) \right|_{H^3}^2 + B^2 |C(t)|_{H^3}^2 + F^2 \int_0^t e^{p_1(s-t)} |C(s)|_{H^3}^2 ds \right. \\ &\quad \left. + G^2 |C_0|_{H^3}^2 \right] + \frac{2\beta_2^2 A}{5\epsilon} \left| \frac{\partial C}{\partial t}(t) \right|_{H^2}^2 \ . \end{aligned}$$

From (42) we have that

$$\frac{d}{dt}\left(\mathbb{E}(E_h(t))\right)$$
$$\leq \tfrac{10\epsilon}{A}\left(\|E_h(t)\|_h^2 + A\,\|D_{-x}E_h(t)\|_+^2 + \tfrac{|F|^2 A}{40 p_1 \epsilon^2}\int_0^t \|D_{-x}E_h(s)\|_+^2\, ds\right) + h^4 K(t)\ ,$$

and taking $\epsilon = \sqrt{\frac{F^2 A}{80 p_1 B}}$ we obtain

$$\frac{d}{dt}\left(\mathbb{E}(E_h(t))\right) \leq \phi \mathbb{E}(E_h(t) + h^4 K(t)\ ,$$

where $\phi = \frac{10\epsilon}{A}$. Finally multiplying by $e^{-\phi t}$ and integrating with respect to t we conclude (31). ■

6. Numerical results

To illustrate the qualitative behavior of the model studied in this paper we present in this section numerical results for the solutions of the initial-boundary value problem (8)-(11) using method (25). We consider in [0,1] a spatial grid $I_h = \{x_i,\ i = 0, 1, .., N\}$ with $x_0 = 0$, $x_N = 1$ and a time grid in [0,1] with $\{t_n,\ n = 0, 1, ..., M\}$ such that $t_0 = 0$ and $t_M = 1$.

In Figure 2 and Figure 3 we plot the numerical results obtained with $C_0(x) = 0.5$, $\alpha = 1$, $D = 1 \times 10^{-15}$, $D_v = 1 \times 10^{-4}$, $E_1 = 8 \times 10^{-5}$, $E_2 = 2 \times 10^{-5}$, $\mu_1 = 1 \times 10^5$, $\mu_2 = 1 \times 10^6$, $\Delta t = 13 \times 10^{-4}$ and $h = 17 \times 10^{-4}$. The two plots present similar behavior. As expected, high stress regions correspond to regions where the concentration is higher.

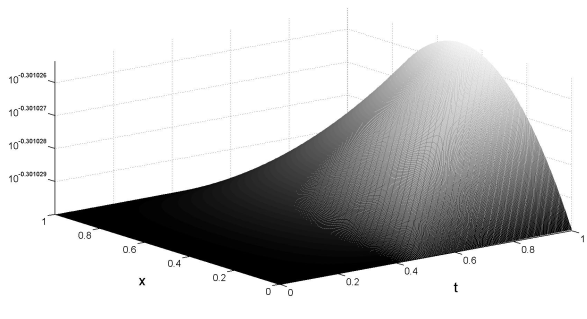

Figure 2. Numerical solution for the concentration

In Figure 4 and Figure 5 we plot a comparison of the numerical results for the concentration and the stress for different values of D at a fixed point of the spatial grid $x = 0.5$ and for a subinterval of the time grid $t \in [0, 1]$.

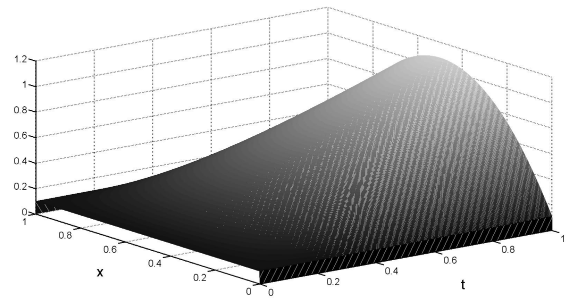

FIGURE 3. Numerical solution for the stress

The remaining constants assume the values previously defined. We observe that the concentration and the stress are increasing functions of the diffusion coefficient. The results are physically sound, because if the liquid diffuses more rapidly into the polymer, the concentration and the stress, also increase more rapidly.

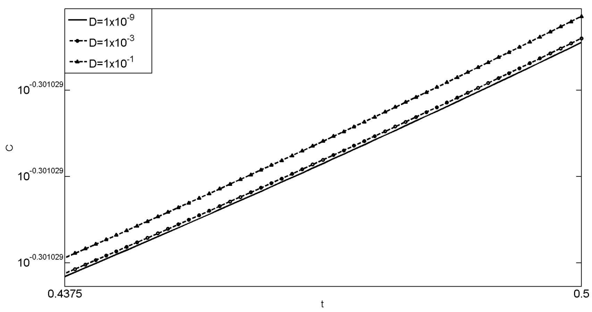

FIGURE 4. Numerical solution for the concentration for different values of D

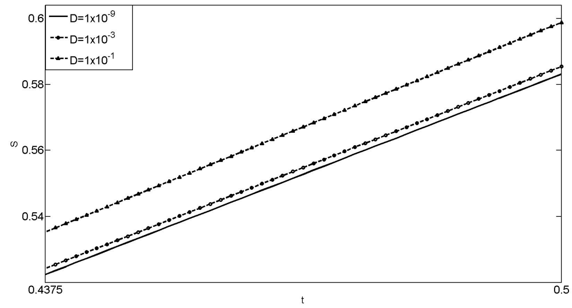

FIGURE 5. Numerical solution for the stress for different values of D

In Figure 6 and Figure 7 we plot a comparison of the numerical results for the concentration and the stress for different values of D_v at a fixed point of the spatial grid $x = 0.5$ and for $t \in [0, T]$. The other constants remain fixed with the same values as before. In this case we observe that the concentration and the stress are decreasing functions of the diffusion coefficient.

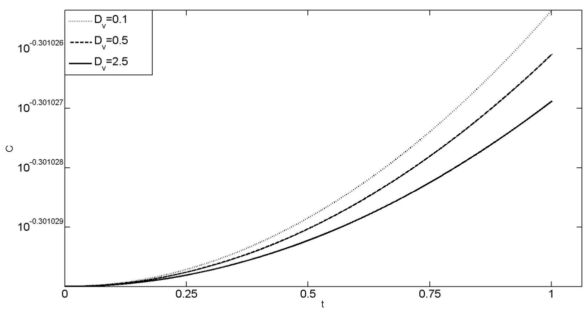

FIGURE 6. Numerical solution for the concentration for different values of D_v

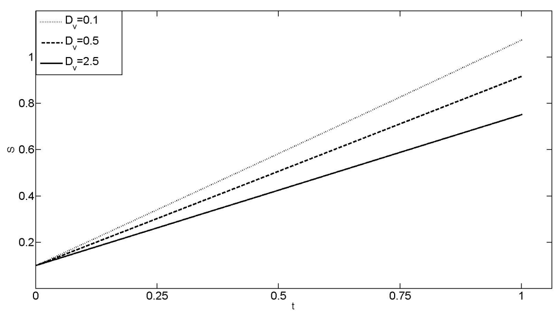

FIGURE 7. Numerical solution for the stress for different values of D_v

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