# Final Report: Reaction-Diffusion in Porous Materials with Porosity-dependent coefficients

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## 1 Introduction

This report analyses the behavior of a coupled diffusion-reaction in a porous medium whose porosity changes with reaction, including the effect of porosity in the diffusion coefficients.

This model is an abstraction of the activity of cells in bone. Although bone is usually thought of as an inert material, it is continuously being resorbed and reformed by bone cells. The first kind of cells, the osteoclasts, travel inside the solid, opening pores. The second kind of active cells, the osteoblasts, come through these pores and attach to the surface, filling the cavities with material.

Although the governing rules for the activity of cells are much more complex, we expect to gain some insight into the role of cell movement inside bone, through the analysis of this simplified model.

## 2 Model formulation

### 2.1 Model equations

The primary quantity is the porosity $\phi$, defined as the volume of pores divided by the total volume. The two other relevant quantities are the amounts of the reactant $C$, which increases the porosity at a rate $r_c$ and $B$, which decreases it at a rate $r_b$. The porosity increases proportionally to the existing volume fraction $1 - \phi$ and to the amount of the reactant $C$. Analogously, the reactant $B$ causes a decrease in porosity proportional to the existing porosity $\phi$. The elements $B$ and $C$ act as catalysts, since they are not consumed in the reaction. They decay espontaneously and proportionally to their respective quantities. Finally, both diffuse with their corresponding diffusion coefficients. In one dimension, this corresponds to the system

$$\frac{\partial \phi}{\partial T} = r_c C(1-\phi) - r_b B\phi \tag{1}$$

$$\frac{\partial C}{\partial T} = D_c(1-\phi)\frac{\partial^2 C}{\partial X^2} - d_c C \tag{2}$$

$$\frac{\partial B}{\partial T} = D_b\phi\frac{\partial^2 B}{\partial X^2} - d_b B \tag{3}$$

where $T$ is the time, $X$ is the spatial coordinate, $r_k$ are the activity coefficients, $d_k$ are the decaying rates and $D_k$ are the diffusion constants.

### 2.2 Dimensionless formulation

In order to get rid of most of the constants, the following transformations will be applied:

$$c = \frac{r_c}{d_c}C \qquad b = \frac{r_b}{d_c}B \tag{4}$$

$$t = d_c T \qquad x = \frac{X}{\sqrt{D_c/d_c}} \tag{5}$$

$$D = \frac{D_b}{D_c} \qquad d = \frac{d_b}{d_c} \tag{6}$$

by which the quantities of cells are replaced by their resorption/formation power (amount per unit time), the time is normalized by the death rate of one of the cell kinds, and the space is normalized by the diffusion of the same kind. The system simplifies to

$$\frac{\partial \phi}{\partial t} = c(1-\phi) - b\phi \tag{7}$$

$$\frac{\partial c}{\partial t} = (1-\phi)\frac{\partial^2 c}{\partial x^2} - c \tag{8}$$

$$\frac{\partial b}{\partial t} = D\phi\frac{\partial^2 b}{\partial x^2} - db \tag{9}$$

where there are only two free parameters.

## 3 Steady-state solution

One of the important characteristics of the underlying physical behavior is the fact that it is, most of the time, at a dynamic steady state, where the activity of $B$'s and $C$'s is in balance. If there is such a state in the model, we are also interested in how the system moves to it.

In the steady state limit, we have

$$c(1-\phi) - b\phi = 0 \tag{10}$$

$$(1-\phi)\frac{\partial^2 c}{\partial x^2} - c = 0 \tag{11}$$

$$D\phi\frac{\partial^2 b}{\partial x^2} - db = 0 \tag{12}$$

Equation (10) expresses the equillibrium described above, and defines uniquely a porosity in the state:

$$\phi = \frac{c}{b+c} \tag{13}$$

$$1 - \phi = \frac{b}{b+c} \tag{14}$$

Substituting (13) into (11) and (12),

$$\frac{b}{b+c}\frac{\partial^2 c}{\partial x^2} - c = 0 \tag{15}$$

$$D\frac{c}{b+c}\frac{\partial^2 b}{\partial x^2} - db = 0 \tag{16}$$

which is a system of nonlinear ODE's in $x$. Since $x$ does not appear, it can be rewritten in terms of $B = \partial b/\partial x$ and $C = \partial c/\partial x$, as

$$C\frac{\partial C}{\partial c} = \frac{c}{b}(b+c) \tag{17}$$

$$B\frac{\partial B}{\partial b} = \frac{d}{D}\frac{b}{c}(b+c) \qquad = 0 \tag{18}$$

which is a system of nonlinear ODE's of first order, which can be solved analytically giving

$$\frac{\partial b}{\partial x} = \pm\frac{1}{\sqrt{3D/d}}\sqrt{b^2(2b/c+3)+k_1} \tag{19}$$

$$\frac{\partial c}{\partial x} = \pm\frac{1}{\sqrt{3}}\sqrt{c^2(2c/b+3)+k_2} \tag{20}$$

Since $b$ and $c$ are non-negative, the solutions above would became unbounded for $x \to \infty$ if the plus sign is used. Similarly, the solutions could become negative if $k_1$ and $k_2$ are non-zero. This reduces the system to

$$\frac{\partial b}{\partial x} = -\frac{b}{\sqrt{3D/d}}\sqrt{2b/c+3} \tag{21}$$

$$\frac{\partial c}{\partial x} = -\frac{c}{\sqrt{3}}\sqrt{2c/b+3} \tag{22}$$

Dividing one by the other, one has

$$\frac{\partial b}{\partial c} = \frac{1}{\sqrt{D/d}}\left(\frac{b}{c}\right)^{3/2}\sqrt{\frac{2b+3c}{2c+3b}} \tag{23}$$

which can be used to trace a relation between $b$ and $c$, independent of $x$.

In Figure 1, paths in the $b \times c$ plane are shown. These paths start at $x = 0$ and are attracted by the point $b = c = 0$ as $x$ increases. The porosity $\phi$ can be calculated directly

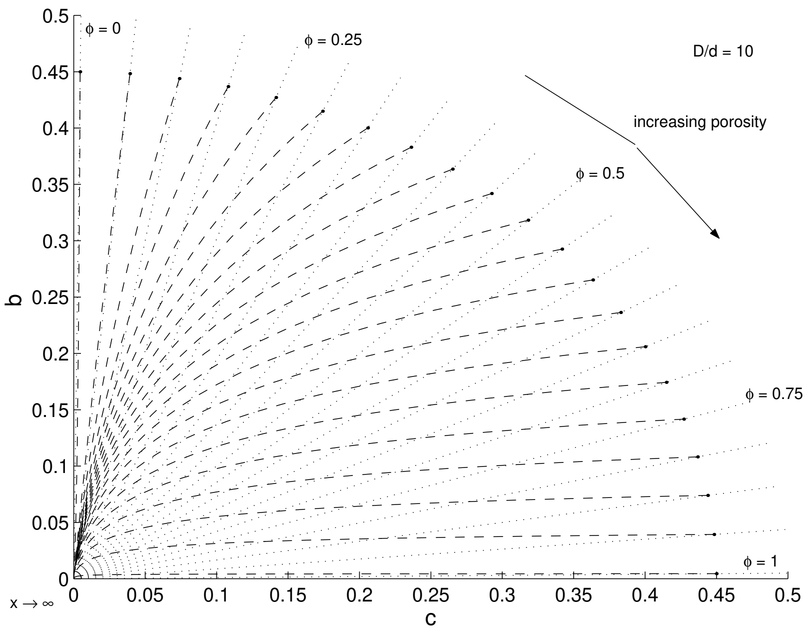


Figure 1: Phase diagram for $b$ and $c$, showing trajectories from the initial state at $x = 0$ to $x \to \infty$. The contours of constant $\phi$ are also indicated.

from $b$ and $c$, and its contours are also shown in the picture. As shown by the trajectories, depending only in the values of the free parameter $D/d$ there will be an assymptotic value for $\phi$ as $x$ goes to infinity.

The behavior in the spatial direction is shown for $b_0 = c_0 = 0.5$ and $D/d = 10$ in Figure 2. Notice that this is the asymptotic behavior, and that although there is an equilibrium value for $\phi$ at large $x$, the values of $b$ and $c$ are so small that effectively any value of $\phi$ is stable for finite time.

# 4 Dynamic behavior

In order to verify the validity of the asymptotic solution found in the previous item, some numerical simulations were performed in order to find the actual porosity profile.

One approximation that was tried was to assume that $b$ and $c$ indeed assume their asymptotic values (or else, that they assume this state much faster that $\phi$) and to solve the initial value problem

$$\frac{\partial \phi}{\partial t} = c_A(1 - \phi) - b_A \phi \tag{24}$$
$$\phi(t = 0) = \phi_0 \tag{25}$$

using the asymptotic values $b_A$ and $c_A$ as constants. Integrating this equation,

$$\phi = \phi_A + (\phi_0 - \phi_A)e^{-(b_A + c_A)t} \tag{26}$$

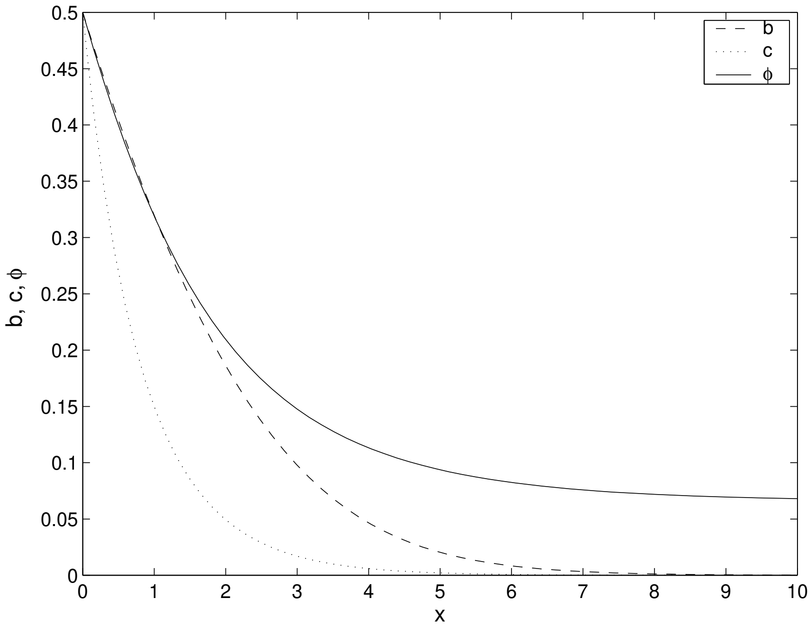


Figure 2: Profiles of $b$, $c$ and $\phi$ as a function of $x$ for $b_0 = c_0 = 0.5$ and $D/d = 10$.

where $\phi_A$ is the asymptotic value of $\phi$. Some values of this solution for different times are compared with the asymptotic solution and with simulations for several values of $t$, in Figure 4.

This approach is flawed, since a different porosity implies different diffusion coefficients at early times, which ruin the approximation. Nevertheless, this is much simpler to simulate and still capture the main aspect of the model behavior.

# 5 Conclusions

We presented the study of a simplified model inspired in a biological phenomenon which happens in bone, in order to acquire a better understanding of the model behavior and to guide the implementation of a biologically consistent approach.

This model allowed the identification of the main invariant quantities, provided the insight of expressing of cells in terms of their resorbing powers and also lead to the definition of the length scales of the problem.

After some simplification hypothesis, the problem became tractable and it was possible to study its behavior in phase space, which gives much more information than numerical simulations. Although the asymptotic behavior is reached very slowly, it was also possible to quantify approximately how the system approaches equilibrium.

Finally, the qualitative features of the model solutions look very promising, indicating that its more detailed cousin will probably be even more successful.

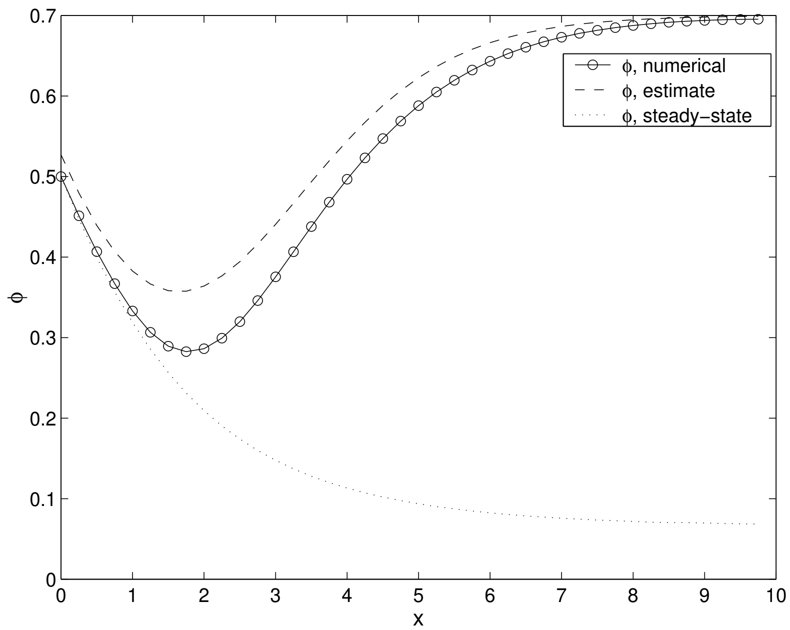


Figure 3: Porosity profiles for an intermediate value of $t$. Steady state solution, numerical simulation and estimate as described in the text.

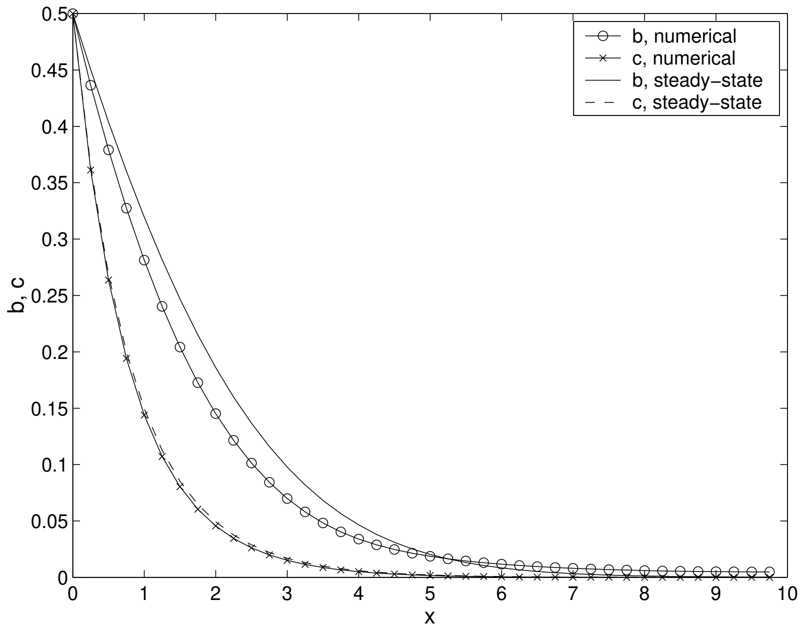


Figure 4: Concentrations of $b$ and $c$ for an intermediate value of $t$. Steady state solution and numerical simulation by the 1-D finite volume method.

## Acknowledgements

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