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H4.SMR/1202-11

"Fifth Course on Mathematical Ecology
including and introduction to Ecological Economics"

28 February - 24 March 2000

# Lecture Notes for a Workshop on

# CONTAMINANT DIFFUSION

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Activity

The purpose of this activity is to work with some examples on the possibility of assessment, using Difference or Differential Equations and the presence of polluting elements in the environment. Numerical schemes will also be discussed.

## 1. A First Example

Let us consider a small lake, formed by a stream, or a river, the flow of which is considered constant. Now this lake is, in some way, important for community, be it water supply, recreation, fishing, flood control. We will consider two types of impact: a discharge of some pollutant into the lake, and a polluting source which has an intermittent or continuous discharge into the lake.
This has become a classic example in Linear First Order Ordinary Differential Equations, and it appears in several different forms, specially in Biomathematics courses. It can also be considered, nonetheless, from a discrete point of view, considering fixed time steps, as weeks, for example. In this case, we would have an equation of the following kind, considering:
**$c_n$**: amount of pollutant in week n (and this can be considered both as mass or as concentration);
**q**: periodic discharge of polluting matter;
**F**: flow of the stream, both into the lake and out of it;
**V**: volume of the lake; and
$\sigma$: weekly decay rate of polluting matter.

In this situation, a discrete approximation of the evolutive process could be given by:

$$c_{n+1} - c_n = - ( F/V ).\, c_n - \sigma.\, c_n + (q/V) \qquad \text{or}$$

$$c_{n+1} = ( 1- F/V - \sigma).c_n + (q/V) = \lambda.\, c_n + (q/V)$$

In case q is null – which means that the periodic discharge has been interrupted, then this becomes a simple geometric progression, indicating that the pollutant will asymptotically go to zero if the absolute value of $\lambda$ is smaller than 1. Of course this very simple to put into a program, but it is an interesting exercise to test different strategies for discharge, using this simple program. For example, q might be a monthly discharge, so for three weeks, q = 0, and on the fourth one, q is a given value. What would be the consequences of this policy? What could be another choice of policy to maintain the concentration cn beneath a certain level?

This model contains certain very strong assumptions, such as the instantaneous dilution of the polluting matter into the whole volume of the lake, and that the flow is constant, something that in the long run is simply not true. Nevertheless, some of these hypotheses can be dropped, making the model better. There is a limit, though: this is a discrete model.

## 2. A First Example again

Let us now consider a continuous problem, in which instead of the weekly values, we have instantaneous rates. Now, the values of the pollutant concentration no longer are constant during the whole week – or considered period – but vary continuously in time: $c = c(t)$. We will then have:

$$\frac{dc}{dt} = -\frac{F}{V}.c(t) + \frac{q}{V}.$$

A first exercise is to check and see if the dimensions agree. And, immediately after, to obtain the analytic solution in those cases in which q is a given constant, or a periodic function. But what is probably happening in lakes in many places is that q is intermittent, meaning that discharges will occur when no one is around, and when agents of environmental protection agencies are around no one assumes the guilt...

We will then have to make use of numerical tools, the most commonly programmed of which are Runge-Kutta methods and variations: MATLAB has a very efficient of these, identified as ODE45 (and a faster and simpler version, ODE23).

Using one of these helps, try to obtain a strategy that might maintain pollutant levels beneath certain limits.

Again, if we consider F to be constant, we might miss the effects of annual droughts, or of the periodic rains. Monsoons, spring thaws or otherwise changes in the environment. With numerical tools, these can be included in the model, and strategies tested.

## 3. The first Example expanded

The limits or the above models become evident as we begin to think about their possible uses. One of the first of these problems is when the lake gets smaller and smaller, and becomes just another part of the stream or river we are considering. How can we study the evolutive aspects of polluting matters being transported downriver? The previous models, with only one compartment (the lake, or dam, as a whole) will not do, since the location of the pollutant is constantly changing. Indeed, in some cases the monitoring can be observed on-line, with local measurements or satellite images, for example.

An interesting idea is presented in Thomann (1996), in which the author describes what he actually did for the North American EPA: He broke the river up into successive compartments, each of which was then considered separately, as was the lake of the first example. In the discrete case, we would have, in each of these compartments, the pollutant arriving from the previous sector of the river, the polluting matter which leaves the compartment continuing downriver, plus possible polluting sources in that particular part of the river. In the discrete case, considering

$\lambda_{i,i+1}$ is the rate of transport of pollutant from compartment **i** to compartment **i+1**;
$\mu_i$ is the decay of the pollutant in compartment **i**;
$\mathbf{c}_i^{(k)}$ is the concentration of pollutant in compartment **i** in time period **k**; and
$\mathbf{q}_i$ is the polluting source in compartment **i**,

we would have (with the obvious adaptations in the first and last compartments)

$$\ldots \rightarrow c_{i-1}^{(k)} \rightarrow c_i^{(k)} \rightarrow c_{i+1}^{(k)} \rightarrow \ldots$$

$$c_i^{(k+1)} - c_i^{(k)} = + \lambda_{i-1,i} \cdot c_{i-1}^{(k)} - ( \lambda_{i,i+1} + \mu_i ).c_i^{(k)} + q_i^{(k)}$$
for i=1,2,...,N and for successive time steps k.

This would give us an equation similar to that of the first point, only this one is written for vectors and not for scalars:

$\mathbf{C}^{(k+1)} = \mathbf{A}.\ \mathbf{C}^{(k)} + \mathbf{q}^{(k)}$, for a given set of values for $\mathbf{q}^{(0)}$, and for matrix A given by

$$A = \begin{bmatrix} 1-\mu_1-\lambda_{12} & 0 & 0 & 0 & ..\ 0 \\ \lambda_{12} & 1-\mu_2-\lambda_{23} & 0 & 0 & ..\ 0 \\ 0 & \lambda_{23} & 1-\mu_3-\lambda_{34} & 0 & ..\ 0 \\ 0 & 0 & \lambda_{34} & 1-\mu_{32}-\lambda_{45} & ..0 \\ \ldots & & & & \\ 0 & 0 & \ldots & \lambda_{N-1,N} & 1-\mu_N-\lambda_{Ne} \end{bmatrix}$$

From the analytical point of view, this is quite a simple equation, since we end up with the calculation of the greatest eigenvalue, but it is probably more interesting to undertake the calculation of the first 40 or 50 vectors, to actually look at what happens in the model. On one hand, we can use

>> [ v d ] = eig(A) (↓) (here we use "↓" for "Enter")

this produces two matrices: one has eigenvectors as its columns, the other has the eigenvalues on the main diagonal.
But it is more instructive to plot successive values of $\mathbf{c}^{(k)}$ to see what the model produces. It is also interesting to discuss what the mathematical results imply in terms of environmental impact, as well as possible consequences.

## 4. A second, continuous Example

What if we need a model in which changes are to be evaluated or measured instantaneously? Instead of a system of Difference Equations, we will need systems of Differential Equations. These equations will keep some similarities with the one seen above, but as in numbers 1 and 2, both analytically and numerically, changes are significant. Whereas in discrete models, convergence is equivalent to having the greatest of the norms of the eigenvalues strictly smaller than 1, this same kind of behavior depends on the eigenvalue being negative, or having a negative real part (since they now appear as exponents of e). For a situation in which we divide a river into successive compartments, as in the previous part, we get:

find $C(t) = (C_1(t), C_2(t), \dots, C_n(t))$, $t \in (0, T]$ such that, for given initial conditions, $C(0) = (C_1(0), C_2(0), \dots, C_n(0))$:

$$\left\{ \frac{dC_i}{dt} = -(\mu_i + \lambda_{i,i+1}).C_i + \lambda_{i-1,i}.C_{i-1} + q_i \right. \text{ for } i = 1,2,\dots,n \text{. Or}$$

$$\frac{d\vec{C}}{dt} = M.\vec{C}(t), \qquad \text{for matrix M given by:}$$

$$\begin{bmatrix} -\sigma_1 - \alpha_{12} & 0 & 0 & 0 & ..\,0 \\ \alpha_{12} & -\sigma_2 - \alpha_{23} & 0 & 0 & ..\,0 \\ 0 & \alpha_{23} & -\sigma_3 - \alpha_{34} & 0 & ..\,0 \\ 0 & 0 & \alpha_{34} & -\sigma_4 - \alpha_{45} & ..0 \\ \dots & & & & \\ 0 & 0 & \dots & \alpha_{n-1,n} & -\sigma_n - \alpha_{ne} \end{bmatrix}$$

From the point of view of analytic results, this is quite straightforward, but numerically we have problems even with this "perfect" analytic solution since we must calculate all eigenvalues – numerically! Now this may be less accurate than using a Runge-Kutta-type method (as in the ODE45 subroutine given by MATLAB). This method was used to obtain, in the case of only 7 compartments, the results shown below. In this case, all $q_i$'s were null, and the first vector, for time $t_0 = 0$, had pollutant only in the first compartment (and one can see that in all others, concentration of the said pollutant is null). The graph illustrates what the text means by suggesting that we "see" what happens:

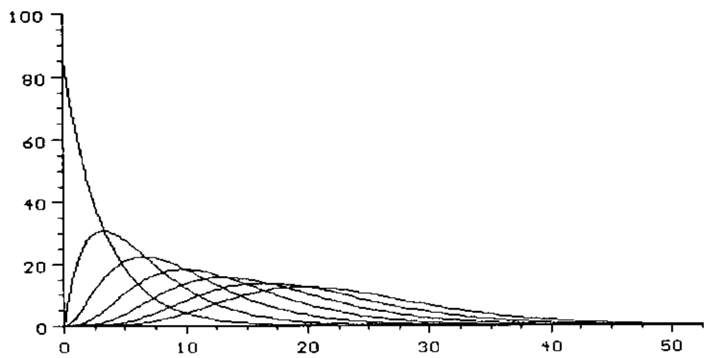

Figure 1: Each curve represents the concentration in one compartment.

In some rivers, this linear choice of compartments is quite enough, since the width of rivers with respect to their length can accept the chosen simplification. In some large ("large" meaning really big ones!) rivers, though, lateral compartments can be chosen, and instead of seeing a polluting matter flow downriver, we can see it spread out at the same time we see it move downriver. In GEORGES (1998), this algebraic effort is detailed, but the resulting system differs in the above mentioned one only in the number of secondary diagonals, since a different interaction is added to that of successive compartments: that of lateral ones as well. What motivated this approach was an oil spill in the Amazon River, in front of the city of Manaus, where most of the electricity is generated by oil.

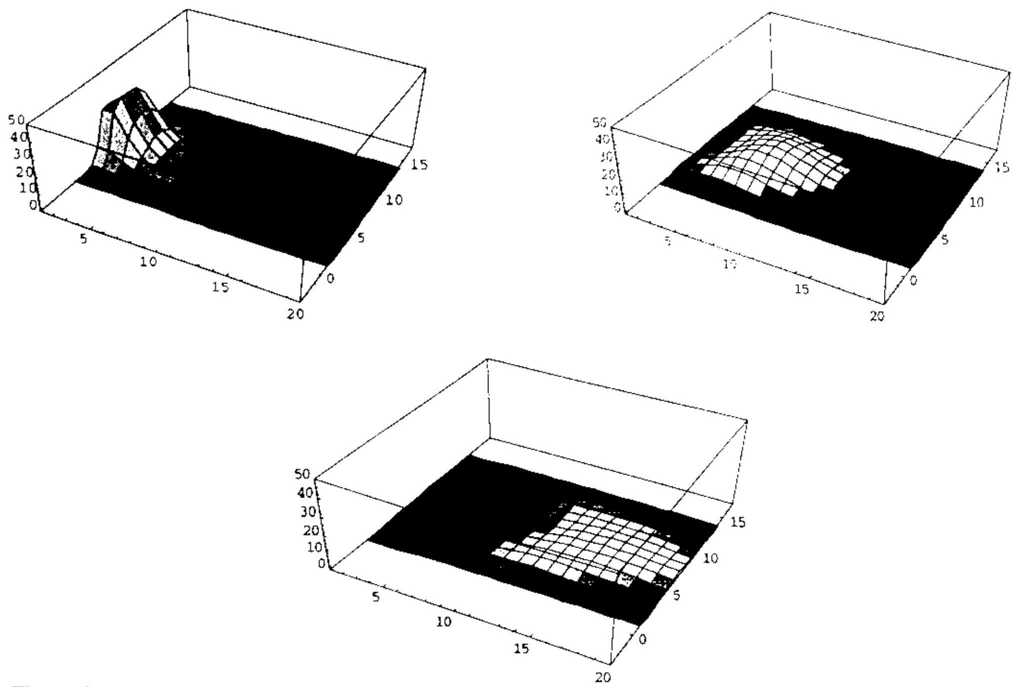


Figure 2: Each graph indicates, in different moments, the concentration of pollutants on the river surface.

There is, in this case a clearly spatial aspect, besides the evident time change. This is given by the choice of compartments, indicating a natural evolution for the type of model we can work with: in this case, besides having only one independent variable, time, having other variables, to describe changes in spatial aspects.

## 5. A diffusion-advection Description

The main mathematical tool here is that of mass continuity:

> *"In a certain region, the rate of change of the variation of the concentration of mass per unit time is equal to the rate of the mass entering the region, minus that which leaves the region, plus what comes from possible sources or leaves due to sinks within the said region, divided by the region volume."*

This is expressed in mathematical terms using concentration $c = c(x, y, z; t)$. We will then have, for a diffusion coefficient $\alpha$, a decay parameter $\sigma$ and a velocity field $V$, in a domain $\Omega \subset R^3$:

find $c = c(x, y, z; t)$ such that

$$\frac{\partial c}{\partial t}(x, y, z; t) = -\operatorname{div}(-\alpha.\vec{J}(x, y, z; t) + \vec{V}.c) - \sigma.c + f(x, y, z; t)$$

for $(x, y, z) \in \Omega \subset R^3$, and $t \in (0,T]$.

What we have here is that the flux considered is not only due to pollutant being transported by a velocity field $\bar{V}(x, y, z; t)$, but also due to diffusion which occurs in a direction which is opposite to the gradient of the studied concentration of polluting matter. Now this diffusion process is considered in the sense given by MARCHUK (1986): the effective diffusion, be it particular or turbulent. Also present is a term representing a sink or a source, given by f( x, y, z; t)

Several texts have the deduction of this equation. Reference here is to the proofs present in EDELSTEIN-KESHET (1987) and in CRANK (1985).

In some situations, the above formulation can be simplified in terms of the geometry of the studied domain. These simplifications do not always (meaning, in fact, "almost never"...) lead to a situation where analytical solutions are easy to obtain. In fact the problem here is the characteristics of domains, of initial conditions, of sources that turn on and turn off, doing away with continuity, for example. The simplifications presented here indicate the numerical tools that can be chosen for convenient approximations of the solution. In cases as these, one many times uses Finite Differences, an approximation choice which depends on regularity of solutions which can be counted upon to exist – the possibility of expanding the solution using some terms of a Taylor polynomial.

Let us consider a one-dimensional version of this problem. In some lakes with a more-or-less constant depth – which can be considered as constant, therefore, and where circulation is very low, we are many times justified in studying the Water column, and repeating what happens in one vertical direction for the whole lake considered as the collection of all columns. In the stationary sense, that is to say, supposing that we can consider changes only in one space variable (which is to be chose as the x-direction!), we get: find $c = c(x)$ such that

$$\alpha.c''(x) + V.c'(x) + \sigma.c(x) = f(x)$$

for $x \in [0, H]$, where H is the constant depth (equivalent to saying that x=0 indicates the surface).

The positive sign of V indicates that the velocity field is in the same direction as that of the x-axis, meaning both point down

We must still get boundary conditions, which might very well be something like:

$$c'(x) = 0 \text{ and } c(H) = 0,$$

meaning no pollutant evaporates, and decay and depth are such that there is never any pollutant in the bottom. Another possibility could be:

$$c(0) = 0 \text{ and } c'(H) = 0$$

which indicates that no pollutant stays on the surface, and no pollutant enters the sediment. An alternative, if a proportion (given by $k$) of the pollutant present does, in fact, penetrate the sediment, could also be given by: $c'(H) = -k.c(H)$

an expression which originates in the von Neumann condition given by

$$-\alpha.\frac{\partial c}{\partial \eta}\bigg|_{\partial\Omega} = p.c|_{\partial\Omega}.$$

A situation that could reasonably justify the use of some numerical method is given if we consider the form of f. In some cases, pollutants are deposited on the surface of these lakes (like acidifying cinders from burnt sugarcane plantations, a very common and unfortunate phenomenon in southern Brazil), and f(x) is given by a constant value for x=0 and is null for any other x in the domain... Similar difficulties arise when we have – from a practical point of view – differences in the water parameters, due, for example, to temperature gradients, where big differences happen for very small variations in the depth x:

$$\alpha(x)=\begin{cases}\alpha_1 \text{ for } 0 \le x \le h_0 \text{ and}\\ \alpha_2 \text{ for } h_0 < x \le H.\end{cases}$$

An exercise which is both interesting and useful is that of changing parameters, coefficients or boundary conditions (taking care to avoid extreme cases...) and "looking" at the numerical results. . The following figures show a first case in which concentration of pollutant decreases to zero as the depth x goes from the surface to the bottom, and in the second figure, with a downward velocity field, an accumulation of polluting matter along the bottom.

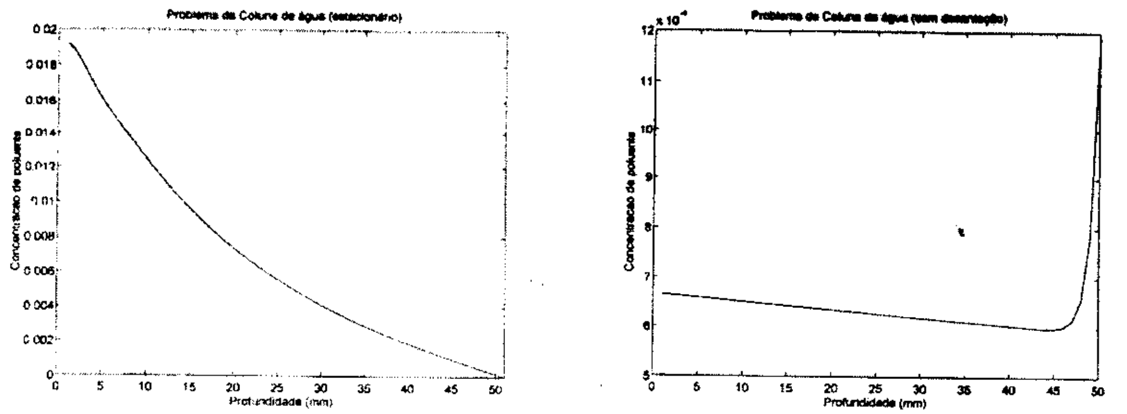


Figure 3: water column example, stationary cases

The next step would be that of including variation in time (and, luckily, MATLAB has a command appropriately called 'movie'!) and plotting successive results to have an idea of the evolutive situation:

Find c = c(x; t), for given c(x; 0) such that

$$\frac{\partial c}{\partial t}=\frac{\partial}{\partial x}(\alpha\frac{\partial c}{\partial x}-V.c)-\sigma.c+f(x,t), \quad \text{para } x\in\Omega\subset R \text{ e } t\in(0,T].$$

the idea is to include the boundary conditions which "fit" the situation we are simulating.

Numerical treatment is that of Finite Differences of second order in the space variables besides Crank-Nicolson in time, also of second order. The following figure includes the time variable t to the space variable x:

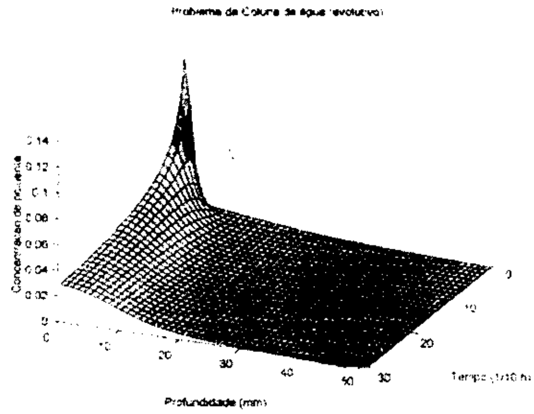

Figure 4: Space and Time: water column.

## 6. Diffusion-advection in 2 dimensions

The general equation presented in the beginning of part 5, which was written for space variables x, y, an z may be considered only in two space dimensions, a simplification which is both necessary and justifiable. For example, considering the presence of surface pollutants in water bodies, such as in the case of an oil spill, it is often the case of an oil slick of several square kilometers, but with a height of a few millimeters – clearly a case in which only the x and y variables need to be included in the model. If, besides, we suppose that the diffusibility is constant, the mentioned equation becomes:

find $c = c(x, y; t)$, for given $c(x, y; 0)$, such that

$$\frac{\partial c}{\partial t} - \alpha \Delta c + \vec{V}.\nabla c + \sigma.c = f(x, y, t), \quad \text{for } (x, y) \in \Omega \subset R^2 \text{ and } t \in (0, T], \quad \text{with}$$

appropriate boundary conditions.

This equation includes the diffusive processes, transport of pollutant due to a velocity field, a term for decay and a polluting source.

References


1. CRANK, J. *The Mathematics of Diffusion*, Clarendon Press, 1985.
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