REACTIVE TRANSPORT IN THE HYDROSPHERE

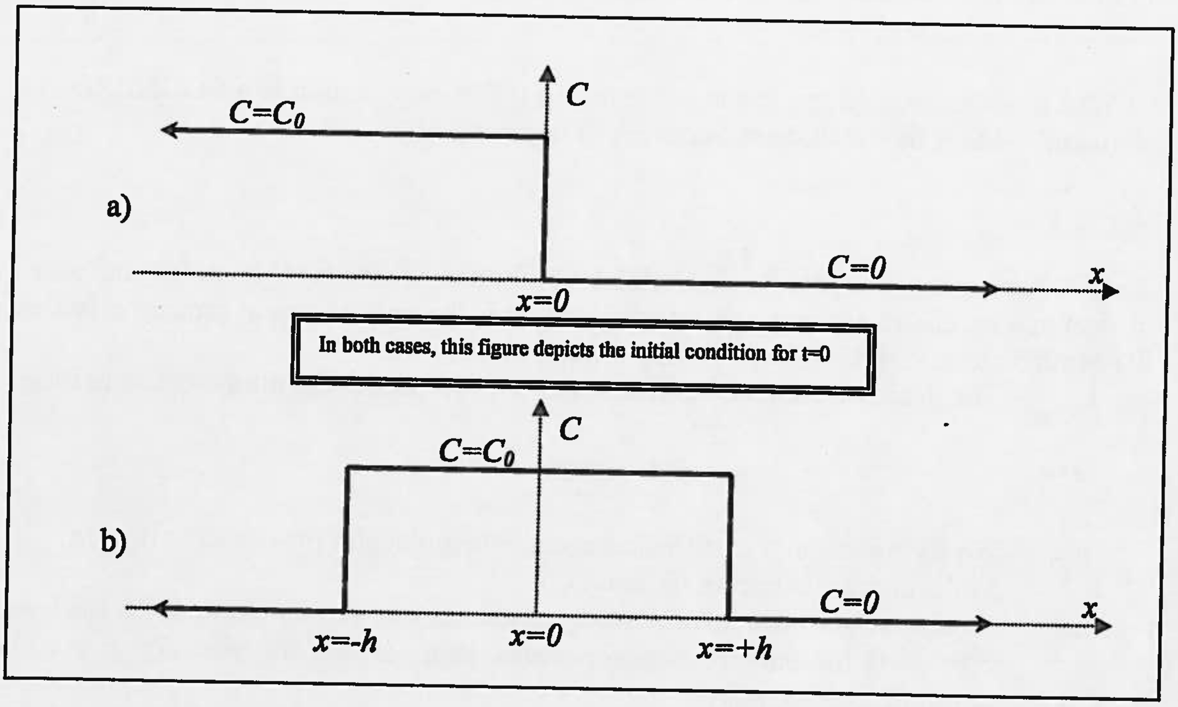
EXAM 16 APRIL 2004

1.

Solve the diffusion equation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$$

subject to the following two extended sources:



Assume that diffusion occurs in an unbounded domain, and recall that the solution for an elementary point source is of the form:

$$C(x,t) = \frac{M}{2\sqrt{\pi Dt}}e^{-\left(x^2/4Dt\right)}$$

You will also need the error function defined as:

$$erf(z) = \frac{2}{\sqrt{\pi}}\int_0^z e^{-u^2}du$$

Sketch the change in concentration profile versus distance as a function of time for the two extended source solutions.

2.

a) Write (i) an explicit and (ii) an implicit scheme for the time-dependent advection-dispersion-reaction equation using a central difference for the advective term:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial x} + kC$$

Explain briefly how you would solve these two discretized equations. How would you solve for the implicit scheme if the reaction term would become nonlinear, i.e.:

$$R = kC^n$$

b) List the set of conservation equations that are required to solve for the flow field in a marine stratified environment (i.e. a system of non-constant density). What are the set of unknowns in this problem?

c) Which method would you use to solve for the diffusion equation in a BOUNDED domain? What is the fundamental concept of this method?

3.

Establish and solve a model for the vertical distribution of nitrate (C in moles/cm^3 pore water) in a sediment, assuming that denitrification is the only chemical process affecting its depth distribution. Use the following assumptions:

i. The denitrification rate is first-order with respect to the nitrate concentration:

$$R = \frac{dC}{dt} = -kC$$

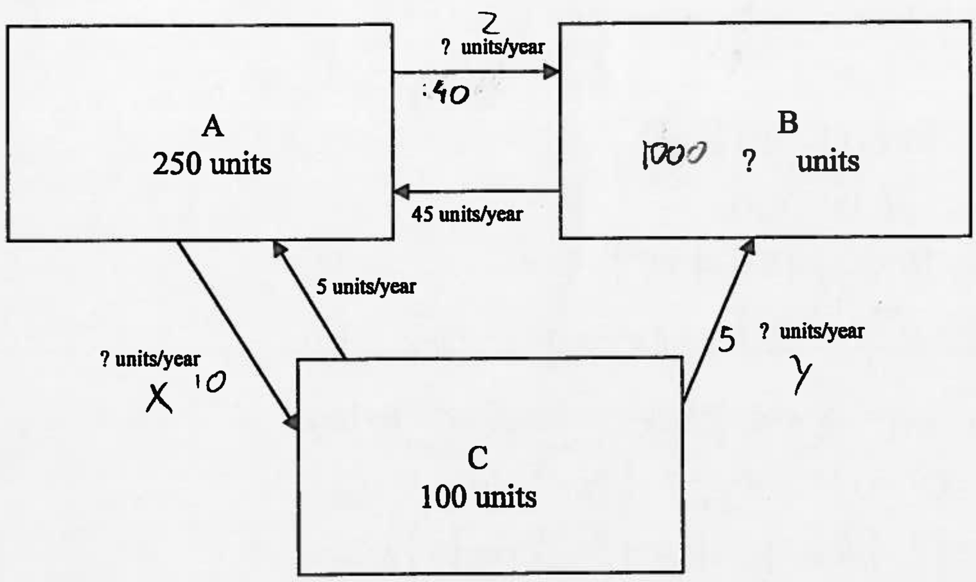
ii. No Bioturbation (i.e. diffusion occurs via molecular processes only with molecular diffusion coefficient D_m);

iii. Compaction, water flow, porosity gradients, etc. can be ignored, i.e. the burial rate ω is the only advection process. Both ω and the porosity ϕ are also constant with depth.

iv. Steady-state diagenesis is achieved

Assume that $C_{x=0} = C_0$ and that $C_{x\to\infty} \to 0$. What is the simplified solution if the advective term (i.e. the burial rate) is very small? In this case, sketch the depth distribution of C when $k >> D_m$ and $k << D_m$

4. Given the following incomplete scheme of reservoirs for a biogeochemical cycle in steady state



And the following incomplete set of linear differential equations describing the same system.

$$\begin{array}{ccc} A\to w & B\text{-}A & C\to A \\ -0{,}2 & & 0{,}05 \end{array}$$

$$\frac{d}{dt}\begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} ? & 0.045 & ? \\ 0{,}16 & -0{,}045 & 0{,}05 \\ 0.04 & 0 & -0{,}1 \end{pmatrix}\begin{pmatrix} A \\ B \\ C \end{pmatrix}$$

$$0{,}05$$

a) Fill in the missing information.
b) Solve the system, by writing the functions that indicate the evolution in time of each of the reservoirs for the system given above.
c) In the case of systems described by non-linear differential equations, describe one quantitative method and one qualitative method that can be used in order to study the stability.
d) Is there any analogy between linear and non-linear systems for studying the stability?
e) Discuss in detail the stability of a system having the following eigenvalues:

$$\lambda_1 = 0; \; \lambda_2 = -3 - i; \quad \lambda_3 = -3 + i; \quad \lambda_4 = \sqrt{2}$$

f) Write an example of eigenvalues and eigenvectors for a system with two different reservoirs that eventually would reach a steady state, where one of the reservoirs ends up with twice as much of the component as the other one. Point out which is which.

5.
a) During the numerical integration of a reactive transport model (RTM), the reaction and the transport subcomponents can be decoupled. Describe two different approaches to combine these parts.

b) What are the residual functions and where are the used during the integration of a RTM?

c) Given the following set of residual functions, calculate one row and one column of the Jacobian and explain what it is used for.

$$f_1 = K_{eq,1} \cdot [H_2CO_3] - [H^+] \cdot [OH^-]$$
$$f_2 = K_{eq,2} - [H^+] \cdot [HCO_3^-]$$
$$f_3 = K_{eq,3} \cdot [H_2CO_3] - [H^+]^2 \cdot [CO_3^{2-}]$$
$$f_4 = \frac{[CO_{2(g)}]^{n+1} - [CO_{2(g)}]^n}{\Delta t} - k_4\left([H_2CO_3]^{n+1} - K_H [CO_{2\,(g)}]^{n+1}\right)$$
$$f_5 = \left([H_2CO_3]^{n+1} + [HCO_3^-]^{n+1} + [CO_3^{2-}]^{n+1} + [CO_{2\,(g)}]^{n+1}\right)/\Delta t - \\ -\left([H_2CO_3]^n + [HCO_3^-]^n + [CO_3^{2-}]^n + [CO_{2\,(g)}]^n\right)/\Delta t$$
$$f_6 = \left([H^+]^{n+1} - [HCO_3^-]^{n+1} - [OH^-]^{n+1} - 2[CO_3^{2-}]^{n+1}\right)/\Delta t - \\ -\left([H^+]^n - [HCO_3^-]^n - [OH^-]^n - 2[CO_3^{2-}]^n\right)/\Delta t$$

d) Explain the difference between the Newton-Raphson method and the LU-decomposition and how they can be used during the integration of a RTM.