A NEW SIMPLE MODEL TO NUMERICALLY SIMULATE REFRESHING PROCESSES IN SALINE AQUIFERS

A. SOTO MECA✉, S.A. GÓMEZ-LOPERA, F. ALHAMA, and C.F. GONZÁLEZ-FERNÁNDEZ

Department of Applied Physics, Technical University of Cartagena. Muralla del Mar Campus, Doctor Fleming s/n, E-30202, Cartagena, Spain.
E-mail: antonio.soto@upct.es

Abstract

A new simple, fast and versatile numerical approach to simulate refreshing processes in saline aquifers is proposed. A convection-dispersion equation with a sorption term is applied to a large aquifer with a step concentration change on one side as the boundary condition. Based on the network simulation method, the spatial finite-differences differential equation (with time as a continuous variable) is used for the design of the model, which is run in the Pspice code. Each term of that equation, whether lineal or non-lineal, is implemented in the model by an unique electrical device belonging to the library of the simulation code, named control current source. In this way, very few devices (five at most) make up the control volume of the model. The programming rules for designing the model file are very simple, even in the case of devices associated to the non-linear addends of the partial differential equation. Applications to refreshing processes are included and the results presented.

Keywords: refreshing, marine intrusion, aquifers, network model.

Introduction

The importance of seawater intrusion phenomena has been emphasized by Appelo and Postma (1999) who have carefully studied this problem (Bear *et al.*, 1999). The salinization of groundwater in coastal aquifers can lead to severe deterioration in the quality of water resources (Oude Essink, 2001). The management of these resources is directly related to climatic changes which can also lead to an increased desertification, as already occurs in the Mediterranean arid zones (Lambrakis and Kallergis, 2002).

The refreshing phenomenon takes place when groundwater of a brackish aquifer, dominated by Na^+ and Cl^- ions, is displaced by freshwater derived from natural recharge, generally dominated by Ca^{2+} and HCO_3,

✉ Corresponding author

after pumping has ceased. Responsible for the refreshing are the cationic exchangers, such as oxyhydroxides, organic matter, and loamy or rocky materials. In the chemical reaction of the exchangers, the Na^+ sorbed on the solid phase is largely replaced by Ca^+, which is liberated, thus changing the composition of the water from a NaCl type to a $CaCl_2$ type (Bear *et al.*, 1999). This ion exchange capacity represents the limiting factor in the recovery, in a reasonable time, of the original water quality. Based on laboratory experiments (e.g. Fidelibus, 2003), seawater intrusion is normally very fast in comparison to the complete recovery of the aquifer, which may last from hundreds to thousands of years.

The non-linearity of the partial differential equation of the diffusion-reaction type for finite aquifers, together with the boundary conditions that define the mathematical model of the refreshing process, mean that it is necessary to use numerical methods to obtain approximate solutions to the problem. Most of the classical numerical methods used by researches are based on the finite-element or finite-difference techniques; however, others, such as the characteristics or random walk methods, which avoid numerical dispersion problems (Oude Essink and Boekelman, 1996), come to the front.

In this paper we solve the refreshing problem by a new technique based on the Network Simulation Method, NSM (2002). The network model of a volume element is designed from the finite differential equation derived from the spatial discretization of the advection-dispersion-sorption equation. In this way, the equations of the model are formally equivalent to finite ordinary differential equations. As in the characteristics method, time remains as a continuous variable. Once the network model is obtained, including the initial and boundary conditions, the numerical solution is obtained from the simulation in the standard computer code for network simulations such as Pspice (1994). The main advantage of the NSM is that the user does not need neither to manipulate the large set of algebraic differential equations connected to each volume element nor to give special attention to the convergence problems. The sophisticated numerical methods integrated in the code carry out this work.

The proposed numerical method has been applied for studying changes of Na^+ concentration in the aquifers of Gouves and Malia in Greece (Lambrakis and Kallergis, 2002). Both long dry periods in recent years and over-pumping resulted in the lowering of groundwater level and seawater encroachment (Malia). The same effects caused a new piezometric regime, with negative water levels (below the sea) in Gouves. The results, directly obtained from the Pspice environment, are shown by means of graphics.

Nomenclature

α_L	dispersivity coefficient (m), $\alpha_L=D_L/v$
b	aquifer thickness (m)
C	capacitor
C	Na^+ concentration (mol/L)
C_1, C_2	Na^+ concentration in the fresh- and the brackish water, respectively (mol/L)
D_L	coefficient of longitudinal hydrodynamic dispersion (m^2/s)
G	control current source associated to the advection term
I	recharge (mm/year)
j	Na^+ flow density (mol/m^2s)
k_d	distribution coefficient (adimensional)

N	total number of cells
q	Na^+ sorpted concentration (mol/L)
R	retardation factor, $R=1+k_d$
R	resistor
t	time (s)
v	pore water flow velocity (m/s)
x	space co-ordinate (m)
$2\Delta x$	thickness of each cell (m)

Subscripts

adv	advection
dis	dispersion
i	cell number (1, 2, …, N)
$i-\Delta x, i, i+\Delta x$	left end, centre and right end of the cell
in, out	entering and leaving
sto	stored

Physical and mathematical models

The problem under study is taken from Appelo and Postma (1999). An infinite 1-D aquifer in which advection, dispersion and sorption processes take place is initially (t=0) separated in two semi-infinite zones, $-\infty<x<0$ and $0<x<\infty$, in which the concentrations are C_1 and C_2, respectively. Far from the contact point (x = 0), this is at $x\rightarrow\infty$ and $x\rightarrow-\infty$, as *t* increases the concentrations C_1 and C_2 do not vary.

Making use of Fick´s law, $j=D_L(\partial C/\partial x)$, the mathematical model is formed by the advection-dispersion-sorption differential equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_L \frac{\partial C}{\partial x} \right) - v\frac{\partial C}{\partial x} - \frac{\partial q}{\partial t} \tag{1}$$

the boundary conditions being

$$C_{(t>0)} = C_{1,}, x = -\infty \tag{2}$$
$$C_{(t>0)} = C_{2}, x = +\infty \tag{3}$$

and the initial conditions

$$C_{(t=0)} = C_{1}, x < 0 \tag{4}$$
$$C_{(t=0)} = C_{2}, x < 0 \tag{5}$$

When is expressed as a lineal function of in the form

$$\frac{\partial q}{\partial t} = k_d \frac{\partial C}{\partial t} \tag{6}$$

were k_d is the distribution coefficient, Equation (1) reduces to

$$(1+K_d)\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left(D_L\frac{\partial C}{\partial x}\right)-v\frac{\partial C}{\partial x} \tag{7}$$

The approximate analytic solution of the problems (Appelo and Postma, 1999) is:

$$C(x,t)=C_2+\frac{1}{2}(C_1-C_2)erfc\left(\frac{\frac{x-vt}{R}}{\sqrt{\frac{4D_Lt}{R}}}\right) \tag{8}$$

where *erfc* is the complementary error function.

Network model

The design of the network starts from the finite difference differential equation derived from the spatial discretization of Equation (7)

$$2\Delta x(1+k_d)\frac{dC}{dt}=\left(\frac{\frac{C_{i+\Delta x}-C_i}{\frac{\Delta x}{D_L}}-\frac{C_i-C_{i-\Delta x}}{\frac{\Delta x}{D_L}}}\right)-v\left(C_{i+\Delta x}-C_{i-\Delta x}\right) \tag{9}$$

The nomenclature of the volume element is shown in Figure 1. Defining the fluxes $j_{dis,in}$ (entering dispersion flux), $j_{dis,out}$ (leaving dispersion flux), $j_{adv,out}$ (leaving advection flux), $j_{adv,in}$ (entering advection flux) and $j_{i,sto}$ (stored flux) in the form:

$$j_{sto,i}=2\Delta x(1+k_d)\frac{dC}{dt}\ ,\ j_{dis,out}=\frac{C_{i+\Delta x}-C_i}{\Delta x}\ ,\ j_{dis,in}=\frac{C_i-C_{i-\Delta x}}{\Delta x} \tag{10}$$

$$j_{adv,out}=vC_{i+\Delta x},\ j_{adv,in}=vC_{i-\Delta x} \tag{11}$$

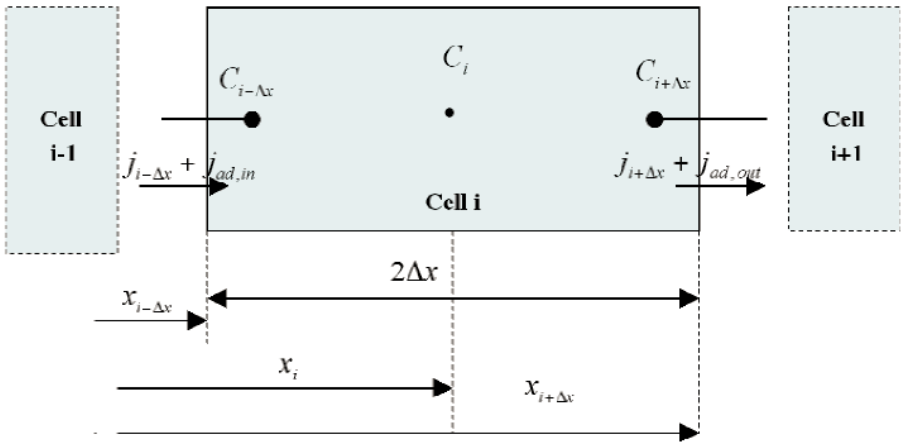


Figure 1. Nomenclature of the volume element.

Equation (9) may be written as an equation balance, which in terms of network analogy (NSM, 2002) is a form of the Kirchhoff current law. On the one hand, Equation (10) allows the electrical devices $R_{i\pm\Delta x}$ and C (two resistors and one capacitor) to be introduced. Resistance and capacitance of these devices are:

$$R_{i\pm\Delta x} = \frac{\Delta x}{D}, \quad C = 2\Delta x(1 + k_d) \tag{12}$$

On the other hand, Equation (11) that refers to advection terms, can be implemented in the network model by two special general proposed devices named "control current sources", $G_{adv,in}$ and $G_{adv,out}$. These generators, which are able to assume any kind on non-linearity, provide a current that may be defined by software. The complete network model for the volume element is depicted in Figure 2. Connecting N of these networks in series and adding the boundary conditions by constant voltage sources at each end, the whole model is completed. The initial conditions are implemented by a suitable voltage at the capacitors (NSM, 2002).

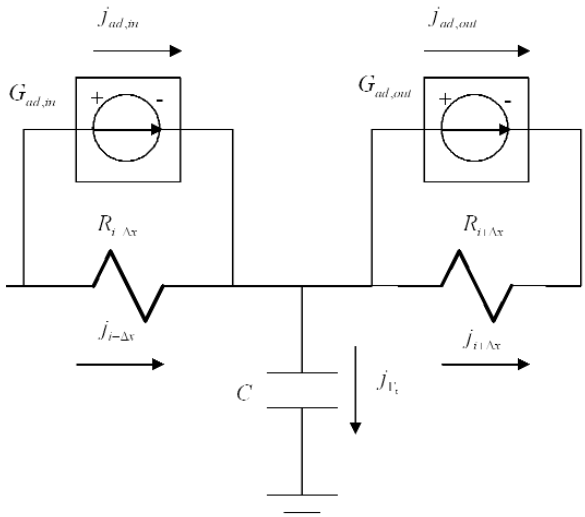


Figure 2. Network model for the volume element.

The simulation, carried out with the Pspice code (1994), the last modification of the code Spice 2 (Nagel, 1975), provides concentrations and separated fluxes at any point of the model. Once the user introduces the code in the model, the numerical results are obtained without further manipulations of the equations. The typical convergence problems are easily solved by appropriate commands provided by the code.

Applications

The proposed model has been applied to simulate two coastal aquifers in Greece: the Neogene formations of Gouves (Grete) and the carbonate aquifer of Malia. To reproduce the boundary conditions, a sufficient

number of volume elements (cells) are implemented to ensure that the Equations (2) and (3) are satisfied, being the real length of the aquifers much smaller than the length of the model. A total of 90 volume elements was implemented in the Gouves aquifer (150 for the Malia), distributed in 40 elements for $x<0$ (69 in Malia), 30 elements for the real length of the aquifer (70 in Malia), and the rest to ensure the boundary condition at $x=+\infty$. The physical characteristics of these aquifers are shown in Table 1.

Table 1. Physical and chemical characteristics of the aquifers.

Gouves aquifer		
Hydraulic characteristics	Symbol	Value
Aquifer thickness	b	30 m
Recharge	I	80 mm/year
Dispersivity	α_L	0.6 m
Initial concentration of Na^+ (brackish water)	C_2	19.03 mmol/L
Initial groundwater quality	C_1	0.38 mmol/L

Malia aquifer		
Hydraulic characteristics	Symbol	Value
Thickness of the aquifer	b	50 m
Recharge	I	399 mm/year
Dispersivity	α_L	0.1 m
Initial concentration of Na^+ (brackish water)	C_2	1.87 mmol/L
Initial groundwater quality	C_1	0.38 mmol/L

For the Gouves aquifer (Figure 3), the freshening time in the hypothetical cases of pumping cessation and natural recharge is very long, being the complete recovery nearly impossible. However, for the carbonate Malia aquifer (Figure 4) this time decreases due to a higher recharge rate, Lambrakis and Kallergis (2002). The network model allows us to identify both the advection and dispersion density fluxes like electric currents. Figures 5 and 6 show the Na^+ total density dispersion and advection fluxes at two typical locations, $x=10$ and 20 m, for both aquifers. Dispersion fluxes are negligible compared to advection fluxes in all cases.

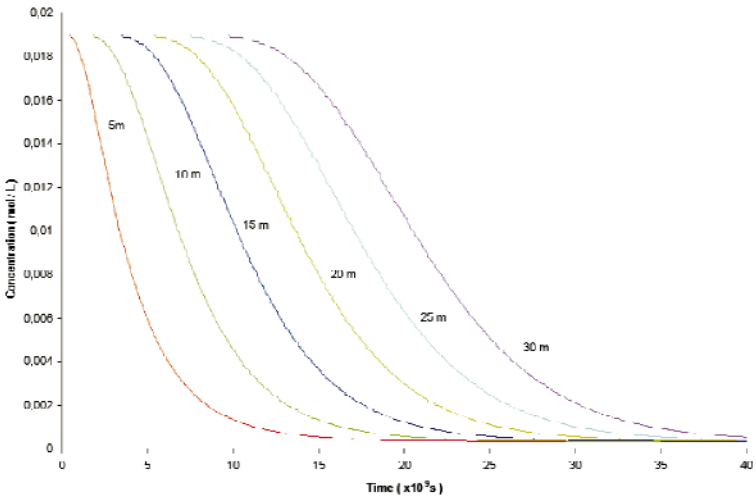


Figure 3. Na^+ concentration-time curves at different locations. Gouves aquifer.

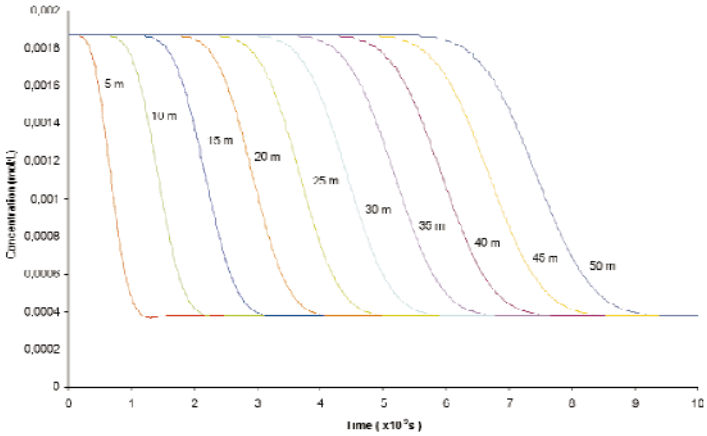
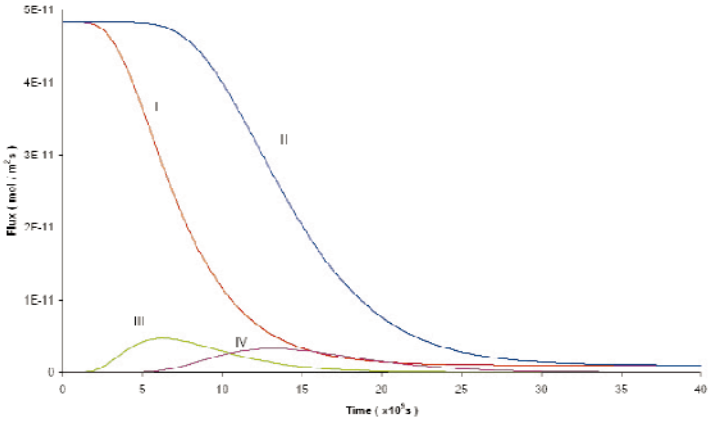


Figure 4. Na^+ concentration as a function of the space co-ordinate. Gouves aquifer.



FigFigure 5. Na^+ advection input density flux at x=10 m (I) and x=20 m (II).
Na^+ dispersion input density flux at x=10 m (III) and x=20 m (IV). Gouves aquifer.

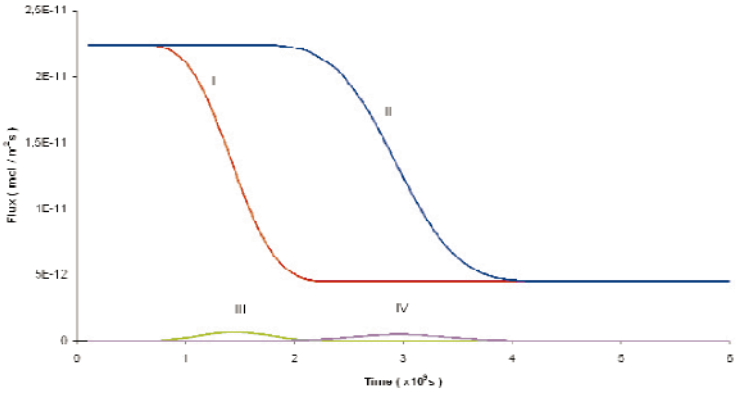


Figure 6. Na^+ advection input density flux at x=10 m (I) and x=20 m (II).
Na^+ dispersion input density flux at x=10 m (III) and x=20 m (IV). Malia aquifer.

Na^+ concentration curves as a function of the space co-ordinate, using time as parameter, are shown in Figure 7 and Figure 8.

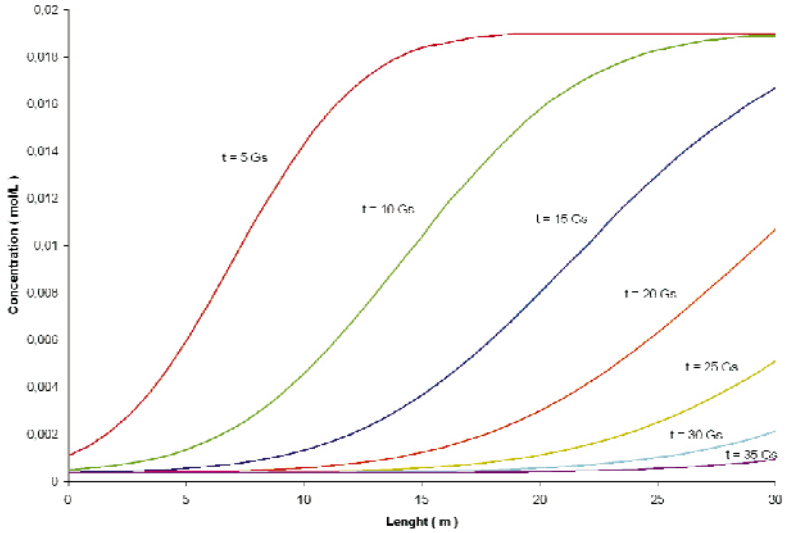


Figure 7. Na^+ concentration as a function of the space co-ordinate. Malia aquifer.

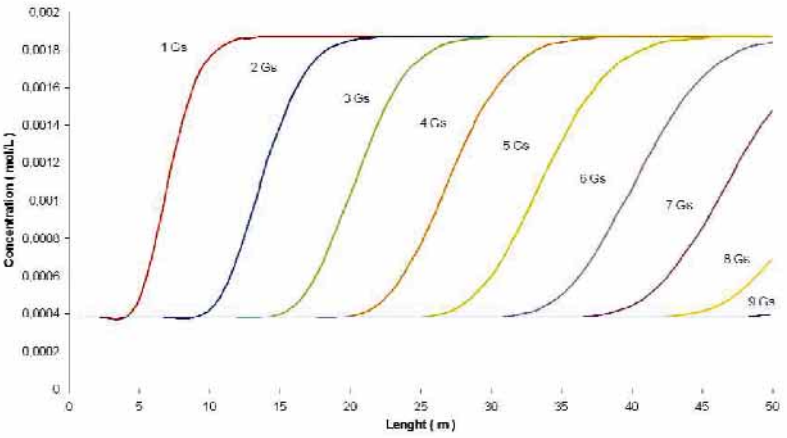


Figure 8. Na^+ concentration-time curves at different locations. Malia aquifer.

In all the simulations carried out, the computing times in a Pentium PC (1GHz) were less than two minutes.

Conclusions

Based on the Network Simulation Method (NSM) a new 1-D model is proposed to simulate the simultaneous advection-dispersion-sorption processes that occur in the refreshing of saline aquifers. The proposed model, whose design is relatively easy due to the few devices that it contains, can be run with small computing time on a PC providing good accuracy. The user does not need to manipulate the finite differential equation or pay attention to the convergence problems once the model is ready. This work is done by the circuit simulation software. The proposed model was applied to the refreshing of Gouves and Malia aquifers and the results compared to those of other numerical methods to test the accuracy of the model.

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