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# A new 2-D numerical model to simulate density-driven flow and solute transport problems

SOTO MECA, A., ALHAMA, F. and GONZÁLEZ FERNÁNDEZ, C.F.
Department of Applied Physics. Escuela Técnica Superior de Ingeniería Industrial
Universidad Politécnica de Cartagena, Campus Muralla del Mar,
30 202 Cartagena, SPAIN

*Abstract:* - The network simulation method (NSM) is here applied, for the first time, to the design of a general purpose model for simulating two-dimensional density-driven flow and solute transport problems through porous media. Although NSM is based on the formal equivalence between physical systems and electrical networks, it is applied to problems of great mathematical complexity such as the coupled non-linear problem here studied. Using the Boussinesq approximation and the streamfunction formulation, the model is applied to solve a problem related with groundwater flow in the vicinity of a salt lake. Simulation is carried out using the digital computer program Pspice.

*Key-Words:* - Density-driven flow, Solute transport, 2-D network model, Network method, Salt lake problem, Porous medium

## 1 Introduction

In contrast to the motion of “ordinary” or “free” fluids that fill the entire space, if a non-flowing solid phase (or one that flows very slowly) is present, the flow obeys Darcy´s law. This is the situation that exists in a porous medium, particularly in groundwater movement near coasts or salt lakes where the fluid density, influenced mainly by salinity, has a substantial effect on the movement of the fluid particles. In addition, solute dispersion processes take place. The unsteady, 2-D mathematical model of these flow systems is adequately represented by:

i) a pair of coupled, nonlinear partial differential equations, generally derived from first principles and whose coefficients may or not may be constant,

ii) the necessary constitutive equations based on experimental studies and currently simplified for mathematical convenience, and

iii) the boundary and initial conditions.

Some problems related to density-driven flow and solute transport are described by Henry [1,2], Elder [3], Voss and Souza [4] and Nield and Bejan [5].

Except in very simplified circumstances, which include the assumption of constant values for the physical properties, the governing equations cannot be solved analytically, and special numerical methods are required.

In this sense, specific codes, such as SUTRA [6] and FAST-C [7] have been developed by different authors. Narayan and Amstrong [8], Fan et al. [9] and Boufadel and Venossa [10] investigate various aspects of this type of problem.

In this work, we present an alternative method based on the network simulation method [11] and using the streamfunction variable. The assumption of Oberbeck-Boussinesq approximation is assumed.

Starting from the finite difference differential equations resulting from the spatial discretization of partial differential dimensionless equations of the mathematical model, a universal electrical network is designed for the elemental control volume or cell. Each addend of the discretized equations is considered as a “current” variable and is implemented in the network by a particular and appropriate device, which are interconnected in such a way that Kirchhoff´s current law is satisfied according to the sign of the addend within the equation.

Since two dependent variables exist, two independent (electrically isolated) circuits appear in the network model of the cell. These cells, in turn, are (2-D) interconnected according to the geometry of the physical model and the linear or non-linear boundary conditions are implemented by simple devices.

An electrical simulation program such as Pspice [12] is used to run (simulated) the model, simultaneously providing the solutions of both streamfunction and salt concentration variables.The proposed model is applied to solving a standard problem of ground water flow in the vicinity of a salt lake [13]. The results are presented in tabulated and graphic form, the latter imported from pspice ambient.

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## 2 Problem Formulation

Assuming the Boussisnesq approach, $\rho \cong \rho_o$, and using the streamfunction ψ, whose relation to specific discharge q (m/s) is given by $\partial\psi/\partial x = q_y$ and $\partial\psi/\partial y = -q_x$, the 2-D coupled equations that define the mathematical model are:

$$\partial[(\mu/k)(\partial\psi/\partial x)]/\partial x + \partial[(\mu/k)(\partial\psi/\partial z)]/\partial z = -g\rho_o\gamma(\partial c/\partial x) \quad (1)$$

$$\varepsilon(\partial c/\partial t) + (\partial\psi/\partial y)(\partial c/\partial x) - (\partial\psi/\partial x)(\partial c/\partial y) - \varepsilon D(\Delta c) = 0 \quad (2)$$

In these equations $\mu$ ($Nm^{-2}s$) is the fluid viscosity, $k$ ($m^2$) the permeability of the porous medium, g ($m^2s^{-1}$) the gravitational acceleration, $\rho$ ($kg/m^3$) the flow density, $\varepsilon$ (dimensionless) the porosity c ($kg/m^3$) the salt concentration and $D$ ($m^2s^{-1}$) the diffusivity. x (m), z (m) and t (s) are the independent variables space and time. To make these equations dimensionless we define the following dimensionless variables:

$x' = x/H$, $z' = z/H$, $t' = t(D/H^2)$,
$q_x' = q_x(H/D)$, $q_y' = q_y(H/D)$,
$\psi' = \psi/D$, $c' = (c - c_o)/(c_s - c_o)$.

which, substituted in equations (1-2) yield

$$(\partial^2\psi'/\partial x'^2) + (\partial^2\psi'/\partial y'^2) = Ra\,(\partial c'/\partial x') \quad (3)$$

$$(\partial^2 c'/\partial x'^2) + (\partial^2 c'/\partial y'^2) - (\partial\psi'/\partial x')(\partial c'/\partial y') + (\partial\psi'/\partial y')(\partial c'/\partial x') = (\partial c'/\partial t') \quad (4)$$

with Ra the Rayleigh number, $Ra = \kappa\,\Delta\rho\, g\, H/(D\mu)$.

## 2 The network model

The first step is to spatially discretize the equations (3-4) and to obtain the finite-difference differential equations in which time remains as a continuous variable.
With $\Delta x'$ and $\Delta y'$ the size of the cell, the resulting discretized equations are:

$$\frac{\Delta}{\Delta x'}\left\{\left(\frac{\Delta\psi'}{\Delta x'}\right)_{out} - \left(\frac{\Delta\psi'}{\Delta x'}\right)_{in}\right\} - \frac{\Delta}{\Delta y'}\left\{\left(\frac{\Delta\psi'}{\Delta y'}\right)_{out} - \left(\frac{\Delta\psi'}{\Delta y'}\right)_{in}\right\} = Ra\frac{\Delta c'}{\Delta x'} \quad (5)$$

$$\frac{\partial c'}{\partial t'} + \frac{\Delta\psi'}{\Delta y'}\frac{\Delta c'}{\Delta x'} - \frac{\Delta\psi'}{\Delta x'}\frac{\Delta c'}{\Delta y'} - \frac{\Delta}{\Delta x'}\left\{\left(\frac{\Delta c'}{\Delta x'}\right)_{out} - \left(\frac{\Delta c'}{\Delta x'}\right)_{in}\right\} - \frac{\Delta}{\Delta y'}\left\{\left(\frac{\Delta c'}{\Delta y'}\right)_{out} - \left(\frac{\Delta c'}{\Delta y'}\right)_{in}\right\} = 0 \quad (6)$$

Subscripts "in" and "out" denote input and output ends of the volume element, respectively.
Each addend of these equations, whatever its form, may be considered as a transport variable (electric current in the network model) that is balanced with the rest of the terms of the same equation according to their algebraic sign. In this sense, the equations themselves may be considered as expressions of Kirchhoff's current, with the balance between the currents of each equation directly assumed by the laws of the circuits.
The network model of the volume element is set up, on the one hand by looking for the electrical devices whose equations are formally equivalent to those of the terms of equations (5-6), and on the other hand by connecting one to the other with the appropriate polarity. Then, the network model of the volume element is connected in series with the rest of the networks, according to the geometry of the medium. Boundary conditions are then implemented using adequate electrical devices [11], while initial conditions are implemented by fixing the voltage of the capacitors.
No mathematical manipulations are required since the simulation software does both the work related to the topological structure of the model (inherent in Kirhhoff's laws) and the work necessary to numerically solve it (inherent with the complex mathematical algorithms implemented in the modern software of circuit simulation). This is one of the important advantages of the proposed method, which basically consists of finding the appropriate device for each term of the discretized equation and connecting them properly. Naming

$$j_{\psi_{i+\Delta x',j}} = \frac{\psi_{i+\Delta x',j} - \psi_{i,j}}{\Delta x'/2} \quad (7a)$$

$$j_{\psi_{i-\Delta x',j}} = \frac{\psi_{i,j} - \psi_{i-\Delta x',j}}{\Delta x'/2} \quad (7b)$$

$$j_{\psi_{i,j+\Delta y'}} = \frac{\psi_{i,j+\Delta y'} - \psi_{i,j}}{\Delta y'/2} \quad (7c)$$

$$j_{\psi_{i,j-\Delta y'}} = \frac{\psi_{i,j} - \psi_{i,j-\Delta y'}}{\Delta y'/2} \quad (7d)$$

$$j_{\psi_{i,j}} = Ra(c_{i+\Delta x,j} - c_{i-\Delta x,j'}) \quad (7e)$$

$$j_{c_{i+\Delta x',j}} = \frac{c_{i+\Delta x',j} - c_{i,j}}{\Delta x'/2} \qquad (8a)$$

$$j_{c_{i-\Delta x',j}} = \frac{c_{i,j} - c_{i-\Delta x',j}}{\Delta x'/2} \qquad (8b)$$

$$j_{c_{i,j+\Delta y'}} = \frac{c_{i,j+\Delta y'} - c_{i,j}}{\Delta y'/2} \qquad (8c)$$

$$j_{c_{i,j-\Delta y'}} = \frac{c_{i,j} - c_{i,j-\Delta y'}}{\Delta y'/2} \qquad (8d)$$

$$j_{1,c_{i,j}} = \frac{(\psi_{i,j+\Delta x'} - \psi_{i,j-\Delta x'})(c_{i+\Delta x',j} - c_{i-\Delta x',j})}{(\Delta x')^2} \qquad (8e)$$

$$j_{2,c_{i,j}} = \frac{(\psi_{i+\Delta x',j} - \psi_{i-\Delta x',j})(c_{i,j+\Delta x'} - c_{i,j-\Delta x'})}{(\Delta x')^2} \qquad (8f)$$

$$j_{C,c_{i,j}} = \Delta x' \frac{dc}{dt} \qquad (8g)$$

eqs. (5) and (6) can be written as

$$j_{\psi_{i+\Delta x',j}} - j_{\psi_{i-\Delta x',j}} + j_{\psi_{i,j+\Delta y'}} - j_{\psi_{i,j-\Delta y'}} - j_{\psi_{i,j}} = 0 \qquad (9)$$

$$j_{c_{i+\Delta x',j}} - j_{c_{i-\Delta x',j}} + j_{c_{i,j+\Delta y'}} - j_{c_{i,j-\Delta y'}} + j_{1,c_{i,j}} - j'_{2,c_{i,j}} + j_{C,c_{i,j}} = 0 \qquad (10)$$

From the point of view of the network model, equations (9-10) can be considered as a Kirchhoff current law at the node (i,j) for the variables water flow and salt concentration. Since there are two dependent variables, two independent circuits must be designed, one for each variable.

The lineal terms (eqs. 7a-d and 8a-d)

$$j_{\psi_{i+\Delta x',j}}, j_{\psi_{i-\Delta x',j}}, j_{\psi_{i,j+\Delta y'}}, j_{\psi_{i,j-\Delta y'}},$$

$$j_{c_{i+\Delta x',j}}, j_{c_{i-\Delta x',j}}, j_{c_{i,j+\Delta y'}}, j_{c_{i,j-\Delta y'}} \text{ and } j_{C,c_{i,j}},$$

are easily implemented in the model by means of eight resistors and one capacitor, respectively, as shown in figure 1. Their respective values are

R=Δx'/2 (=Δy'/2) and

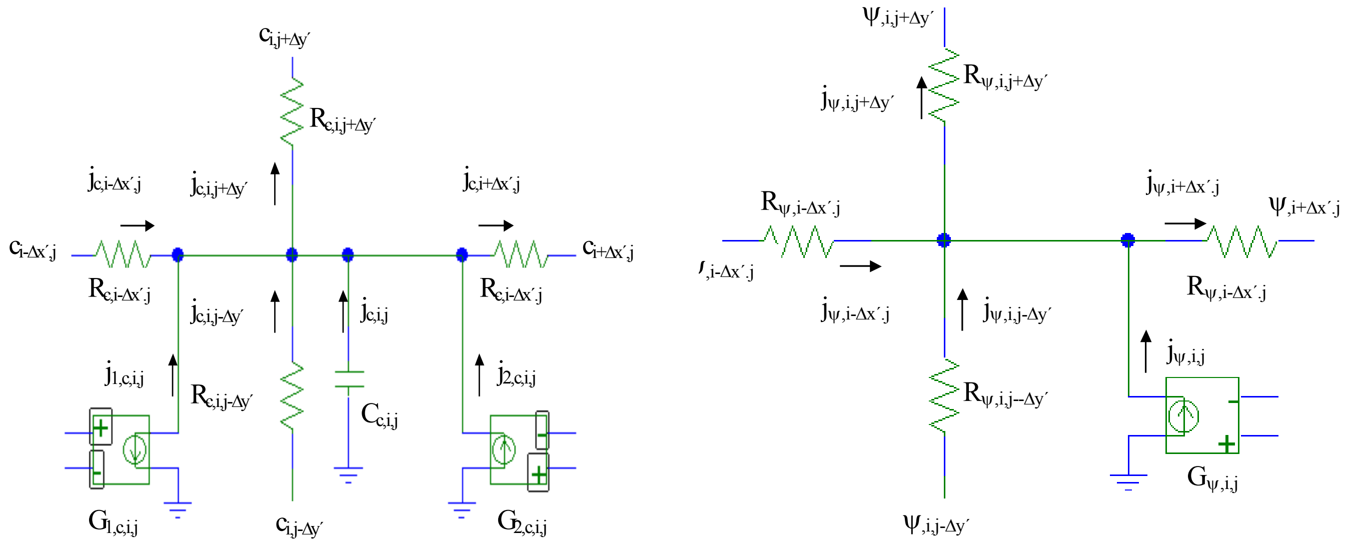
C= Δx'.

The non-lineal terms

$$j_{\psi_{i,j}},\ j_{1,c_{i,j}} \text{ and } j'_{2,c_{i,j}}$$

are all implemented by special devices known as controlled current sources, $G_{\psi_{i,j}}, G_{1,c_{i,j}}$ and $G_{2,c_{i,j}}$, respectively, figure 1.

The output of this source may be specified by software, writing it as a function of the values of the (one or two) dependent variables in a particular point of the medium at each instant. In this sense, any kind of continuous mathematical function may be assumed in the specification of G.




a) b)

Figure 1. Network model of the volume element.
a) streamfunction variable,
b) saltwater concentration variable

Finally, the boundary conditions are easily implemented in the model by means of simple devices.
For example, a first class boundary condition (Diritchlet) requires a constant voltage source, while a second class boundary condition (Neumann) requires a constant current source for the non-homogeneous condition or an infinite (value) resistor for the homogeneous case. These devices are connected to the boundary of the volume elements where the condition applies, figure 3.
Once the network model is completed, its simulation is carried out in Pspice [12]. The handling of this code for idealized situations is easy and "user-friendly". Since very few devices make up the network, very few programming rules are needed. Besides, the possibility exists of designing the network by sketching, using the option "schematics" generally included in the software of circuit simulation.

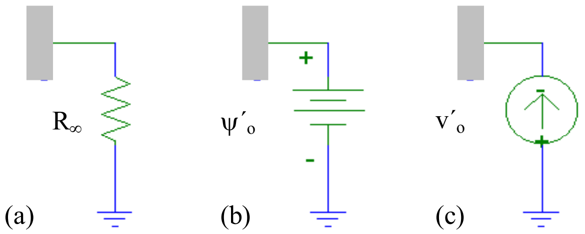



Figure 2. Network devices for the boundary conditions. (a): Neumann (homogeneous) (b) Diritchlet, (c) Neumann (non-homogeneous)

## 3 Application

The following application is based on the real case of the (salt lake) Pilot Valley studied by Fan et al. [9] using the SUTRA code. The model region, schematically shown in figure 3, is a vertical cross-section (vertical axis parallel to direction of gravity, positive upward)
bounded by impermeable strata at the base of the aquifer and by the water table at the top. The salt lake is located on one side of the model. The values of the parameters are (see figure 3):

$H' = 1$ (height of the aquifer, dimensionless)

$L' = 10$ (length of the aquifer)

$A' = 6$ (recharge and zero concentration zone )

$B' = 4$ (no recharge zone)

$C' = 1.6$ (outflow zone)

$D' = 2.4$ (saturated concentration zone)

$Ra = 100$ (Rayleigh number)

$v'_o = 6.5$ (boundary velocity)

$\psi'_o = -39$ (prescribed streamfunction)

while the boundary and initial conditions are:

$\psi' = \psi'_o$, $\partial c'/\partial y' = 0$, $y' = 0$

$\psi' = \psi'_o$, $\partial c'/\partial x' = 0$, $x' = 0$ and $x' = 10$

$\partial\psi'/\partial y' = v'_o$, $c' = 0$, $0<x'<6$, $y' = 1$

$\partial\psi'/\partial y' = 0$, $\partial c'/\partial y' = 0$, $6<x'<7.6$, $y' = 1$

$c' = 1$, $\partial\psi'/\partial y' = 0$, $7.6<x'<10$, $y' = 1$,

$c' = 0$, $t' = 0$

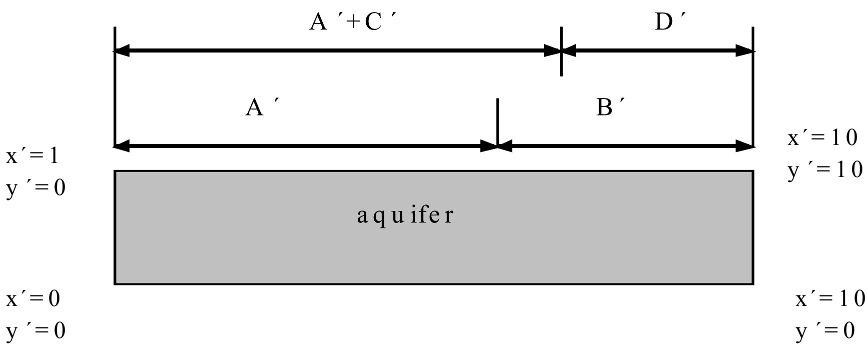



Figure 3. Geometry of the problem

A total of 80 volume elements in the horizontal direction and 40 in the vertical direction are used. Figure 4 and 5 show the unsteady values of ψ′and c′ at typical locations. The order of magnitude of the unsteady duration is 0.5. The stationary values for ψ′and c′ are point in Table 1 and 2, respectively.

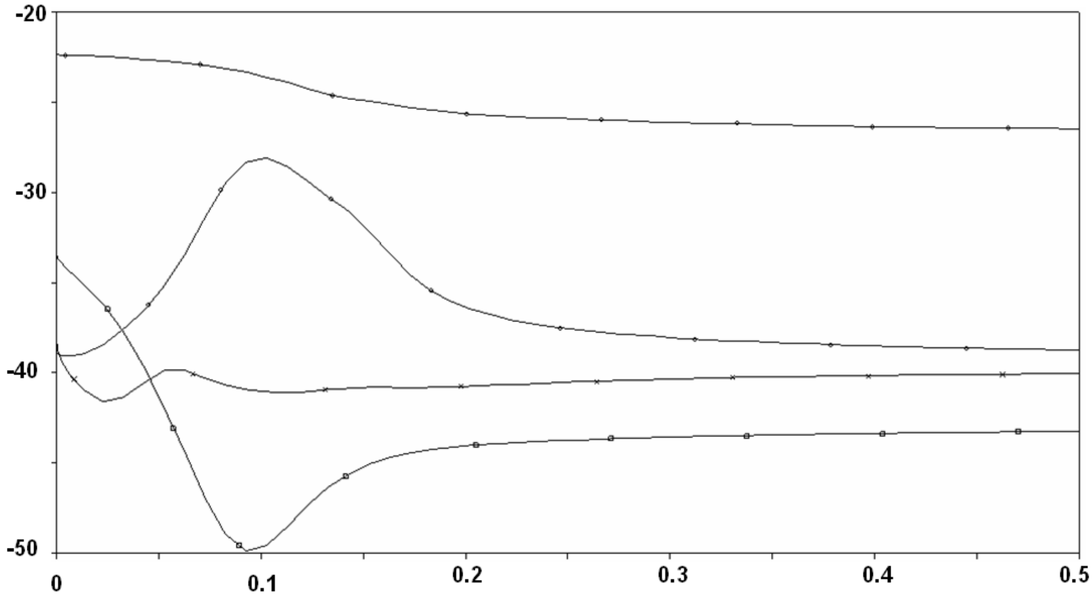



Figure 4. Unsteady streamfunction (dimensionless).
(a): (x′,y′) = (5.5,0.5); (b): (9,0.5); (c): (8,0.5); (d): (6.5,0.5)

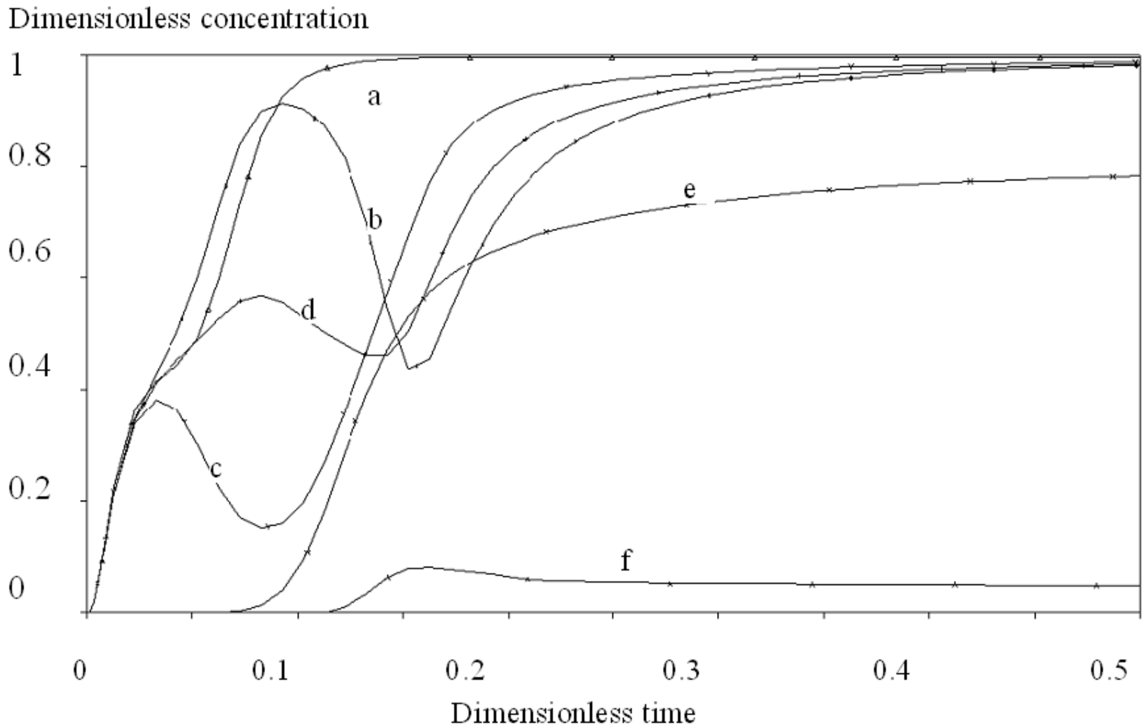



Figure 5. Unsteady salt concentration (dimensionless)
(a): (x′,y′) = (9,0.75); (b): (10,0.75); (c): (9.5,0.75);
(d): (9.75,0.75); (e): (6.5,0.75); (f): (5.75,0.75);

| x´ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| y´ = 0.25 | - 38.5 | - 36.8 | - 35.2 | - 33.5 | - 32.0 | -35.0 | - 41.8 | - 40.2 | - 39.2 | - 38.8 |
| y´ = 0.50 | - 38.0 | - 34.8 | - 31.4 | - 28.0 | - 24.9 | - 26.5 | - 43.7 | - 41.2 | - 39.4 | - 38.7 |
| y´ = 0.75 | - 37.5 | - 32.5 | - 27.5 | - 22.5 | - 17.5 | - 15.8 | - 44.5 | - 42.0 | - 39.5 | - 38.6 |

Table 1. Steady values of streamfunction at typical locations
Dimensionless time: 0.4

| x´ | 5.5 | 6 | 6.5 | 7 | 7.5 | 8 | 8.5 | 9 | 9.5 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| y´ = 0.25 | 0 | 0.610 | 0.930 | 0.966 | 0.985 | 0.992 | 0.990 | 0.982 | 0.967 | 0.954 |
| y´ = 0.50 | 0 | 0.250 | 0.885 | 0.953 | 0.983 | 0.994 | 0.993 | 0.986 | 0.973 | 0.962 |
| y´ = 0.75 | 0 | 0 | 0.800 | 0.933 | 0.979 | 0.996 | 0.996 | 0.993 | 0.995 | 0.978 |

Table 2. Steady values of salt concentration

It can be appreciated that both streamfunction and salt concentration undergo appreciable changes during the non-steady period but they go smoothly to the steady value as time increases.

## Conclusions

From the stream function formulation and based on the network method, a new efficient numerical model has been designed for the solution of unsteady 2-D density-driven flow and solute transport processes in porous media. Two independent circuits in each volume element are implemented, one for the fluid flow variable and one for the salt concentration variable. The coupling between equations is carried out by a current source, whose output is easily defined by software in a easy way. The model is run in a network simulation code Pspice. An application is made to simulate groundwater flow in the vicinity of a salt lake. Computing times are relatively small using a PC.

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