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THE MIXING-CELL TRANSPORT MODEL

A finite difference approach for solving the convection-dispersion equation

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I N H O U D

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INTRODUCTION	1
1. ANALYTICAL SOLUTION OF THE CONVECTION-DISPERSION EQUATION	2
2. MIXING-CELL CONCEPT	3
2.1. Description	3
2.2. Stability	4
2.3. Precision and numeric dispersion	5
2.4. The mixing-cell concept as a numeric series	6
3. EXAMPLES	7
4. CONCLUSION AND RECOMMENDATIONS	9
LITERATURE	10
APPENDIX	

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INTRODUCTION

In groundwater quality models one often uses the convection-dispersion equation that describes the transport of solutes through a porous medium as a result of water movement and dispersion. For a 1-dimensional system this equation is written as follows

$$\frac{\partial c}{\partial t} = -v \frac{\partial c}{\partial x} + D \frac{\partial^2 c}{\partial x^2} \quad (1)$$

where c = concentration at point x at time t

v = actual water velocity inside the pores

D = dispersion coefficient

Eq. (1) is often extended with a decomposition and an adsorption term. In the present approach, however another concept for solving water quality problems will be followed. The transport of solutes will be separated from the reactions of the solutes. This report deals with the transport part which is formulated by means of eq. (1) and is called the mixing-cell concept.

The water quality part dealing with adsorption, complex formation, precipitation etc. will be treated separately. The advantage of separating solute transport and chemical reactions is that one can describe the reactions in detail with one system of mass balances. The time dependent transport terms are then excluded.

1. ANALYTICAL SOLUTION OF THE CONVECTION-DISPERSION EQUATION

Eq. (1) is a one-dimensional parabolic partial differential equation with c as a function of x and t . A well known method for solving this equation is the method of characteristics. This method implies the following transformation of x and t into u and w :

$$u = x - vt \quad (2a)$$

$$w = t \quad (2b)$$

u and w are called the characteristics of eq. (1).

The substitution transforms the coordinates x and t into a moving coordinate system that moves with the same velocity as the water. Substituting eq. (2a) and (2b) into eq. (1) yields:

$$\frac{\partial c}{\partial w} = D \frac{\partial^2 c}{\partial u^2} \quad (3)$$

This is the well known diffusion or heat-flow equation. In the literature several solutions are given.

For example, the solution with the following boundary conditions:

$$c(0, w) = c_f \quad (\text{feed}) \quad (4a)$$

$$c(u, 0) = c_i \quad (\text{initial}) \quad (4b)$$

gives

$$c = c_i + \frac{1}{2}(c_f - c_i) \operatorname{erfc}\left(\frac{x-vt}{2\sqrt{Dt}}\right) \quad (4c)$$

For studying the early stages of the process the complete solution is found with aid of Laplace transformations. According to CRANCK (1964) the solution is:

$$c = c_i + \frac{1}{2}(c_f - c_i) \left\{ \operatorname{erfc}\left(\frac{x-vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{vx}{D}\right) \operatorname{erfc}\left(\frac{x+vt}{2\sqrt{Dt}}\right) \right\} \quad (4d)$$

The difference between eq (4d) and (4c) is called the reflection term. This term describes the process in the region $x < vt$, that is the leftside of the moving coordinate system. This reflection term will diminish with increasing time and increasing front penetration.

2. MIXING-CELL CONCEPT

2.1. Description

Neglecting the second order term of eq. (1) gives eq. (5):

$$\frac{\partial c}{\partial t} = -v \frac{\partial c}{\partial x} \quad (5)$$

The backward explicit finite difference approach of eq. (5) is called the mixing-cell concept. The mixing-cell concept will give the same solution as the analytical solution of eq. (1).

Rewriting equation (5) in terms of Δx and Δt using the mixing-cell concept gives:

$$\frac{c(x,t+\Delta t) - c(x,t)}{\Delta t} = -v \frac{c(x,t) - c(x-\Delta x,t)}{\Delta x} \quad (6a)$$

Rearranging yields:

$$c(x,t+\Delta t) = c(x,t) - \frac{v\Delta t}{\Delta x} \{c(x,t) - c(x-\Delta x,t)\} \quad (6b)$$

or

$$c(i,j+1) = (1 - \frac{v\Delta t}{\Delta x}) c(i,j) + \frac{v\Delta t}{\Delta x} c(i-1,j) \quad (6c)$$

Equation (6c) is illustrated in Fig. 1.

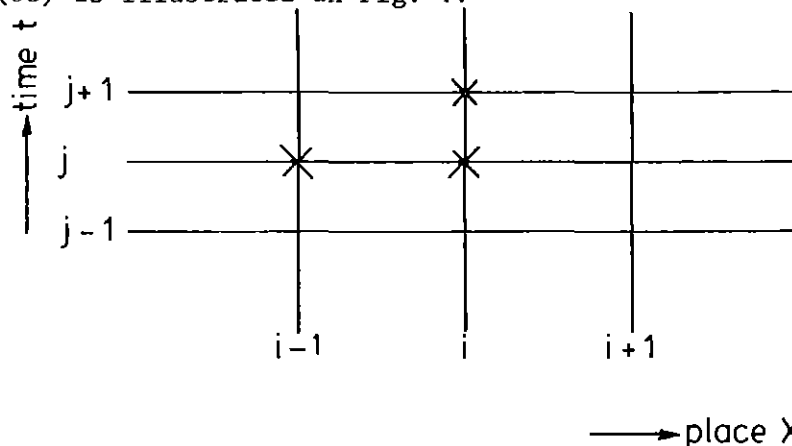


Fig. 1. The i - j grid and the position of the coefficients of equation 6b and 6c

2.2. Stability

The factor $\frac{v\Delta t}{\Delta x}$ is called the mixing ratio. Eq. (6c) describes the mixing of water in compartment i with water coming from compartment $i-1$. The quantity of inflowing water is controlled by the factor $v\Delta t$ and the quantity of remaining water with $x - v\Delta t$. Dividing by the volume of layer i yields the mixing ratio $\frac{v\Delta t}{\Delta x}$.

Take:

- the solution of eq. (6a) at time t is c_x^t
- and \tilde{c}_x^t as the correct solution of eq. (5)
- the difference between the real solution and the calculated one as ϵ_x^t

$$\epsilon_x^t = c_x^t - \tilde{c}_x^t \quad (7)$$

The elements of ϵ_x^t can be described with a fourrier analysis as a function of x (see KAN, 1982):

$$\epsilon_x^t = \gamma_t e^{i\beta x} \quad (8)$$

Substitution of eq. (7) into (6a) gives:

$$\frac{\tilde{c}_x^{t+\Delta t} - \tilde{c}_x^t}{\Delta t} + \frac{\epsilon_x^{t+\Delta t} - \epsilon_x^t}{\Delta t} = -v \frac{c_x^t - c_{x-\Delta x}^t}{\Delta x} - v \frac{\epsilon_x^t - \epsilon_{x-\Delta x}^t}{\Delta x} \quad (9a)$$

Substituting eq. (8) into eq. (9a) and rearranging yields:

$$\frac{\gamma_{t+\Delta t} - \gamma_t}{\Delta t} = \frac{-v\gamma_t}{\Delta x} (1 - e^{-i\beta\Delta x}) \quad (9b)$$

Rearranging gives eq. (10):

$$\frac{\gamma_{t+\Delta t}}{\gamma_t} = 1 - \frac{v\Delta t}{\Delta x} (1 - e^{-i\beta\Delta x}) \quad (10)$$

Stability will occur when:

$$\left| \frac{Y_{t+\Delta t}}{Y_t} \right| \leq 1 \quad (11a)$$

or

$$-1 \leq 1 - \frac{v\Delta t}{\Delta x} (1 - e^{-i\beta\Delta x}) \leq 1 \quad (11b)$$

$$0 \leq \frac{v\Delta t}{\Delta x} \delta \leq 2 \quad (11c)$$

It will be sufficient when $\frac{v\Delta t}{\Delta x} \leq 1$ to obtain stability, because $-1 \leq e^{-i\beta\Delta x} \leq 1$ and thus $0 \leq \delta \leq 2$.

2.3. Precision and numeric dispersion

The finite difference approach with equation (6a) yields infact terms of a Taylor polynomial. The complete Taylor polynomial for the left and right hand side are given in eq. (12a) and (12b):

$$\left(\frac{dc}{dx} \right)_t = \frac{c(x) - c(x-\Delta x)}{\Delta x} + \frac{\Delta x}{2!} \frac{\partial^2 c}{\partial x^2} - \frac{(\Delta x)^2}{3!} \frac{\partial^3 c}{\partial x^3} + \dots \quad (12a)$$

$$\left(\frac{dc}{dt} \right)_x = \frac{c(t+\Delta t) - c(t)}{\Delta t} - \frac{\Delta t}{2!} \frac{\partial^2 c}{\partial t^2} - \frac{(\Delta t)^2}{3!} \frac{\partial^3 c}{\partial t^3} - \dots \quad (12b)$$

Substitution of eq. (12a) and (12b) in (6a) gives with neglection of powers of Δ :

$$\frac{c(x, t+\Delta t) - c(x, t)}{\Delta t} - \frac{\Delta t}{2!} \frac{\partial^2 c}{\partial t^2} \approx -v \frac{c(x, t) - c(x-\Delta x, t)}{\Delta x} - \frac{v\Delta x}{2!} \frac{\partial^2 c}{\partial x^2} \quad (13a)$$

or

$$\frac{\partial c}{\partial t} \approx -v \frac{\partial c}{\partial x} + \frac{\Delta t}{2!} \frac{\partial^2 c}{\partial t^2} - \frac{v\Delta x}{2!} \frac{\partial^2 c}{\partial x^2} \quad (13b)$$

using $\frac{\partial^2 c}{\partial t^2} \approx v^2 \frac{\partial^2 c}{\partial x^2}$ (see Appendix 1)

gives

$$\frac{\partial c}{\partial t} = -v \frac{\partial c}{\partial x} + \left(\frac{v^2 \Delta t}{2} - \frac{v\Delta x}{2} \right) \frac{\partial^2 c}{\partial x^2} \quad (13c)$$

The precision of this finite difference approach is equal to an error of the second order! This error is called numeric dispersion.

Comparing eq. (13c) with eq. (1) yields:

$$D \cong \frac{v^2 \Delta t}{2} - \frac{v \Delta x}{2} \quad (14)$$

Summarizing; the error that is made by using the mixing-cell concept for eq. (5) is of the second order. This error, i.e. the numerical dispersion, depends on the values chosen for Δx , Δt and v . So numerical solution of eq. (5) yields a solution for eq. (1), if the values for Δx , Δt and v are chosen in such a way that the 'numerical dispersion' equals the actual dispersion.

2.4. The mixing-cell concept as a numeric series

Take equation (6c) and write the mixing ratio $\frac{v \Delta t}{\Delta x}$ as α :

$$c(i, j+1) = (1-\alpha) c(i, j) + \alpha c(i-1, j) \quad (15)$$

Assume the following boundary conditions:

$$c(0, j) = c_f \quad \text{the feed concentration}$$

$$c(i, 0) = c_i \quad \text{the initial concentration}$$

For a system of N layers the following response can be calculated:

$$c(i, j) = 0 \quad \text{for} \quad j < i \quad \text{and} \quad 0 < i \leq n \quad (16a)$$

and

$$c(i, j+1) = \sum_{k=0}^{j-i-1} \binom{k+i-1}{i-1} \alpha^i (1-\alpha)^k c_f + \sum_{k=j-i}^{j-1} \binom{j-1}{k} (1-\alpha)^k (\alpha)^{j-k-1} c_i \quad (16b)$$

$$\text{for} \quad j > i \quad \text{and} \quad 0 < i \leq n$$

3. EXAMPLES

Comparing the mixing-cell concept with the analytical solution for a chosen example gives the following result. Take the concentration of the feed solution as unity and the initial concentration zero.

$$v = 5 \text{ cm/day}$$

$$l = 100 \text{ cm (column length)}$$

$$\Delta x = 10 \text{ cm}$$

$$\Delta t = 1 \text{ day}$$

$$\alpha = \frac{v\Delta t}{\Delta x} = 0.5$$

$$N = \frac{l}{\Delta x} = 10$$

$$D = \frac{-v^2\Delta t}{2} + \frac{v\Delta x}{2} = \frac{-25}{2} + \frac{50}{2} = +12.5 \text{ cm}^2/\text{day}$$

The breakthrough curve i.e. the concentration at $x = l$, is plotted in the Fig. 2 and 3.

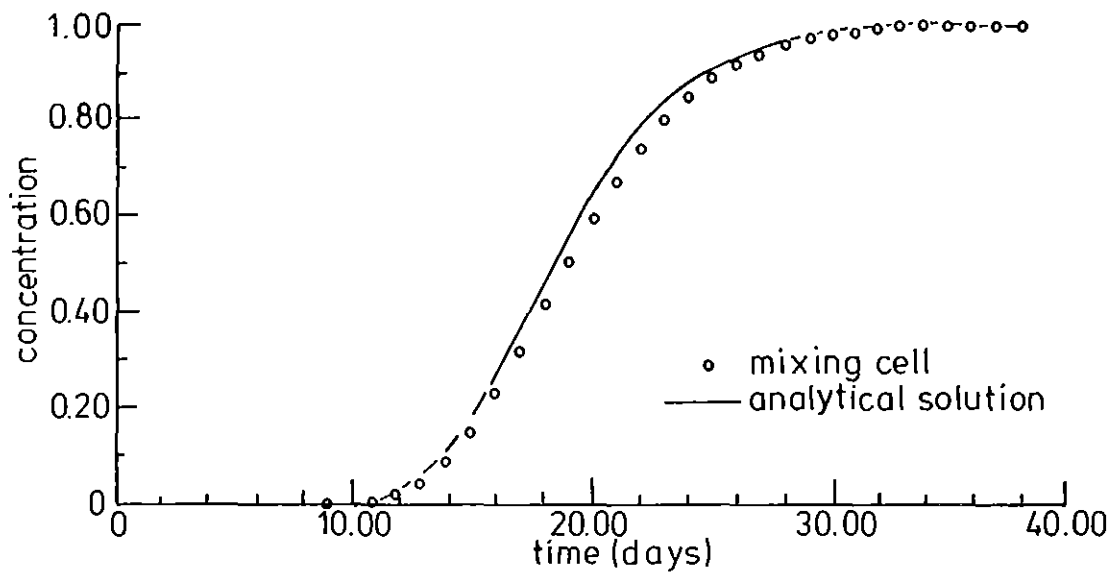


Fig. 2. The results of the mixing-cell model versus the analytical solution of eq. (4d)

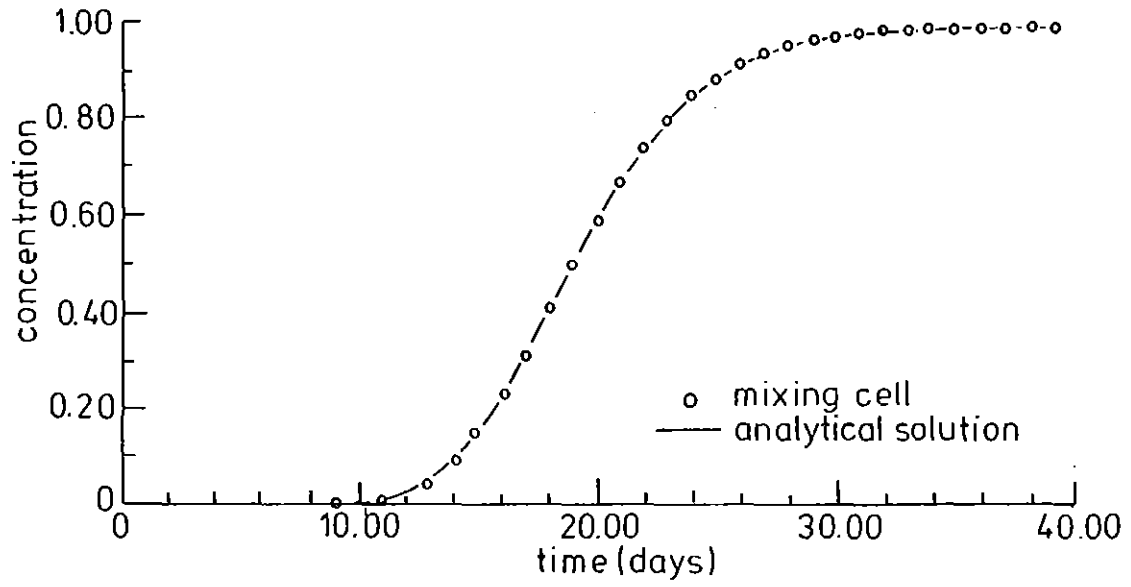


Fig. 3. The results of the mixing-cell model versus the simple analytical solution of eq. (4c)

4. CONCLUSIONS AND RECOMMENDATIONS

The mixing-cell concept is an explicit backward finite difference approach of the transport equation $\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = 0$. The precision of the method is of the second order which means that in fact the convection-dispersion equation is solved.

It is illustrated that the results of the mixing-cell model coincide with the analytical solution (eq. 4c), provided that the reflection at the boundary does not effect the breakthrough curve:

- the first term of the analytical solution (eq. 4d) is identical with the concentration front calculated with the mixing-cell model (if $D_{\text{num}} = D_{\text{act}}$);
- the second term of the analytical solution (eq. 4d) describes the concentration in the early stages of the process (see for instance BOLT, 1982). This phenomena is not described with the mixing-cell concept;
- for larger times the mixing-cell concept fits quite well with the analytical solution.

The advantage of separating transport of solutes from the chemical reactions of the solutes will be illustrated in following reports. Two examples will be referred too. GROENENDIJK (1984) described the combination of the mixing-cell model with the ion exchange of Na, Ca and Mg.

VAN OMMEN (1984) showed the application of the mixing-cell concept to a two dimensional groundwater problem.

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Recapitulating the transport equation (5):

$$\frac{\partial c}{\partial t} = -v \frac{\partial c}{\partial x} \quad (1)$$

According to the definition of differential analysis:

$$\frac{\partial^2 c}{\partial t^2} = \frac{\partial}{\partial t} \left(\frac{\partial c}{\partial t} \right) \quad (2)$$

Substituting eq. (1) into (2) yields:

$$\frac{\partial^2 c}{\partial t^2} = \frac{\partial}{\partial t} \left(-v \frac{\partial c}{\partial x} \right) = -v \frac{\partial^2 c}{\partial t \partial x} \quad (3)$$

Rewriting eq. (3) and substituting eq. (1) gives:

$$\frac{\partial^2 c}{\partial t^2} = -v \frac{\partial}{\partial x} \left(\frac{\partial c}{\partial t} \right) = -v \frac{\partial}{\partial x} \left(-v \frac{\partial c}{\partial x} \right) = v^2 \frac{\partial^2 c}{\partial x^2} \quad (4)$$