

Numerical Simulation of Chemical and Nuclear Contamination Transport in Aquifers and its Possible Application for the Control of Environmental Impacts due to Mining Activity

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ABSTRACT

The paper describes a simulating method for ground water contamination originating from industrial and mining activity.

The finite difference model simulates heat, mass and solute transport. The applied stochastic method for dispersion provides more accurate solution of mass transport modelling.

This method gives a more realistic approach of chemical processes in an aquifer depending on temperature.

INTRODUCTION

The protection of the quality of underground water resources is of great importance even for mining. Two main forms of contamination endangering the aquifers can be distinguished by their origin:

- contamination from the surface
- contamination from underground

TYPES OF CONTAMINATION FROM THE SURFACE

The contaminations from the surface can be listed as follows:

- contamination from precipitation, when rainfall impacted by air pollution filtrates into the unconfined aquifers,
- agricultural contamination caused by animal keeping and chemicals of plant cultivation,
- sanitary landfills,
- industrial waste disposals with or without direct contact

with the water table and industrial waste waters of un-effective treatment,

- contamination from the surface waters: when contaminated water flows are in hydraulic connection with aquifers and the gradients are directed to the aquifer.

CONTAMINATION FROM UNDERGROUND

Contaminations from underground can be accounted as follows:

- contamination from abandoned open pits or deep mine sites: when leakage occurs from old mine sites, Existing potential contamination sources which get contacted with aquifers and change the flow system because of mining discharges.

- Contamination caused by rock solidification or sealing. In this case different physical or chemical materials /natural or artificial/ are injected into the soil or rock mass /e.g. during the sealing with electric filter a big quantity of the sulphate is leached into the aquifers.

- "Thermal effect" can disturb the natural conditions of the aquifer when hot water waste is reinjected after utilization. The disposal of the geothermal waste water with high salt concentration can contaminate the aquifers too.

THE SIMULATION MODEL

The governing equations of the simulation model of finite difference method are as follow:

$$\frac{d}{dt} \int_V \frac{S}{g} P dV = - \int_A \rho \vec{v} \cdot \vec{n} dA + \int_V G_f dV \quad /1/$$

$$\frac{d}{dt} \int_V C dV = \int_A \frac{D}{Rd} \vec{\nabla} C_k \cdot \vec{n} dA - \int_A C_k \frac{\vec{v}}{Rd} \cdot \vec{n} dA + \int_V G_{sz} dV \quad /2/$$

$$\frac{d}{dt} \int_V (\rho C)_M T dV = \int_A K_M \vec{\nabla} T \cdot \vec{n} dA - \int_A \rho C_f T \vec{v}_d \cdot \vec{n} dA + \int_V G_h dV \quad /3/$$

where:

S: specific storage

g: acceleration due to gravity

P: pressure

ρ : density /in function of pressure and temperature/

\vec{v} : flow velocity

G_f : mass flow /sink or source/

C^k : concentration
 D^k : dispersion tenzor
 $D = dv + D^x$ /4/
 d : dispersivity
 D^x : coefficient of molecular diffusion
 R_d : retardation factor
 \vec{n}^d : normal vector over an area A
 G_{sz} : yield of contamination
 C_M : heat capacity of the water-rock mediae

$$\rho C_M = \phi \rho_f C_f + (1-\phi) \rho_s C_s \quad /5/$$

where:

ϕ : rock porosity
 ρ_f : fluid density
 C_f : heat capacity of fluid
 ρ_s : density of rock matrix
 C_s : heat capacity of rock

K_M : heat conductivity
 T^M : temperature
 G_h : heat source

The simplified equation of the impulse equilibrium is given by the Darcy law:

$$\vec{V}_d = - \frac{k}{\mu} \nabla P - \rho \vec{g} \quad /6/$$

where:

k : permeability
 μ : dynamic viscosity

Equations /1/ /2/ and /3/ are interaction by the hydraulic pressure, the temperature, and parameters depending on the water quality and the convective term.

The spatial gradient between nodes are assumed with linear approach as

$$\nabla P = \frac{P_m - P_n}{D_{n,m} + D_{m,n}} \quad /7/$$

The permeability, heat conductivity, fluid density and the concentration at the boundary of nodes /interfaces/ are calculated with weighted harmonic mean values. This

method ensures the continuity of the flow at the interface.

CALCULATION OF FLOW AND HEAT TRANSPORT

The mass and heat transport can be calculated by equations /1/ and /3/. These phenomena are simulated in case examples for practical uses, e.g. thermal water utilization with recirculation /5/ and the change in the condition of Héviz thermal springs /6/. The results of this simulation have met the accuracy requirements of the engineering practice.

SOLUTE TRANSPORT CALCULATION

The distribution of concentration of chemical components in the water can be represented by the distribution of a finite number of discrete particles. This particle can move in two ways: it is moved by the ground water flow to the direction of main seepage and a secondary random movement appears in transversal direction. This random dispersion is described by distribution curves specified according to the length of flow in function of dispersivity.

The displacement parallel to the downstream is calculated by the finite difference method. The transversal movement is described by a stochastic dispersion model presented by Bear /1/ and Fried /3/. A "random walk" solute transport model for groundwater quality evaluations was published at first by Prickett et al. /8. 9./ The movement of a particle is determined as follows:

The movement of a particle is shown in Figure 1, where the steady flow and longitudinal dispersion is supported in direction x. The original particle position x, y changes to a new one /x₂, y/ according to its velocity during a time increment Δt . Then the particle moves to position /x₃, y/ because of random dispersion in direction +x or -x. The value of the random walk distance is described as:

$$S_r = \sqrt{2 d_l \cdot V_x \cdot \Delta t} \cdot A/0/ \quad /8/$$

where:

- S_r : the magnitude of random movement
- d_l : longitudinal dispersion coefficient
- V_x : velocity of direction x
- Δt : time increment
- A/0/: random factor - a number between -6 and +6, drawn from a normal distribution of numbers having a standard deviation of 1 and a mean of zero.

A more general case is illustrated in Figure 2, where the flow direction is not aligned with the x-y coordinate axes and the longitudinal dispersion is taken into account. The effect of the transversal dispersion can be calculated in the same way. During the simulation process both longitudinal and transversal dispersion is considered simultaneously.

ASSUMPTIONS

In the development of the model the following assumptions were applied:

- Darcy's law describes the fluid movement in an adequate manner.
- The rock and the fluid are in thermal equilibrium at any given time.
- Energy changes due to the compressibility, acceleration and viscous dissipation of the fluid can be neglected.
/7/
- Diffusion terms have been considered as follow: /2/
 - "ordinary diffusion" characterized by diffusion coefficient D
 - diffusion due to water head difference.
- Neglected diffusion terms are:
 - thermo-diffusion induced by temperature difference,
 - induced diffusion due to some external force /e.g. electric force, ion migration/.
- The mixing of waters of different concentrations is perfect and considered as short time event inside the node compared with flow process velocity.
- The reversible adsorption-desorption is neglected.
- Dynamic viscosity is independent on the pressure and water quality.
- The model employs the one-dimensional theory of Terzaghi to calculate the deformation of the medium.

JOB SETUP

The model grid

Two or three-dimensional grid can be used. No restrictions for size number, shape and connections of nodes are existed. Each node is specified with its geometric data.

Parameters

Some fluid properties are determined as function of pressure and/or temperature. The density is expressed as function

$$\rho = a_1 + a_2 T + a_3 T^2 + a_4 P + a_5 P^2 \quad /9/$$

/7/

The dynamic viscosity is considered as with function of temperature described by Juhász, J. /4/

The specification of the heat parameters of the fluid /heat capacity, conductivity and initial hydraulic pressure and temperature of nodes/ is required.

The model can be applied for 50 rock types with different properties, but this limit can be exceeded according to the requirement. The following parameters for each rock type must be specified:

- code number of rock type
- permeability
- density
- specific storage
- porosity
- heat capacity of rock
- heat conductivity of the rock matrix.

Local or regional anisotropy for arbitrary rock types can be prescribed.

The retardation factor is used to characterize the change in the solute concentration caused by chemical reactions /adsorption, organic fixation, etc./ in the medium. Chemical reactions between the dissolved constituent and the medium tend to retard the movement of the constituent relative to the groundwater velocity.

The retardation of a concentration front is described by relation /9/

$$\frac{v}{v_c} = R_d \quad /10/$$

where:

- v : interstitial velocity of the groundwater
- v_c : velocity of the $\frac{c}{c_0} = 0,5$ in the concentration front
- R_d : retardation factor

Factor R_d must be specified in the model as input datum. Radioactive decay may be added if desired. The initial concentration of contamination for the nodes and/or for the source of contamination over the area, respectively,

are required as input parameters.

Boundary conditions

Most of the boundary conditions desired for practical uses can be applied in the model. These are as follow:

- nodes with fixed pressure
- changing pressure in space and time
- nodes with fixed temperature
- changing temperature in space and time
- mass sink and source with constant flow rate
- mass sink and source with flow rate changing in time
- heat sink and source with constant value
- heat sink and source with changing in time
- contamination source with constant value
- contamination source with changing value in time
- quickly acting contamination
- constant mass flux at the boundary.

Mass and solute transport processes can be modelled with boundary conditions mentioned before. Iteration parameters adequate for calculations are specified on the input list.

Presentation of output

The output contains all information pieces including important parameters, which determine the character of the task to be solved which are necessary for experts.

Items of the input lists are as follow:

- water level
- water head
- depression relative to the initial conditions
- temperature
- change of temperature from the initial state
- water yield of dewatering and injection
- concentration
- volume of contamination discharge and recharge
- density
- total heat and mass flow across the boundaries.

EXAMPLE PROBLEMS

Three example problems illustrate how the computer code is applied. The system to be modelled consists of grid of 25 nodes and is determined with fixed pressure boundary condition on each side. The grid covers on area of 0.25 km², with node size of 100x100 meters.

The network is presented in Figure 3. The main parameters applied in each version are listed below:

- specific storage of rock matrix: 9.10^{-3} 1/m
- porosity: 0.015
- fluid density: 1000 kg/m³
- relative altitude of node above sea level: 0.0
- temperature of water and rock medium: 10 C⁰
- dynamic viscosity of fluid: 0.00133 Pas
- initial water head: 100 m above sea level.

A very simplified model with symmetrical geometry and closed boundary was used to investigate the processes more easily, although the model has no restriction with regard to the geometrical and boundary conditions. The change of all contaminants dissolved was modelled in the test examples, however, any of the water quality components can be applied.

Version No. 1

In this case a momentary contamination combined with water recharge at the some place of the system was applied. At the opposite side of grid some water discharge is supposed. The simulation time is 170 years, and the output lists are printed by ten years. The rate of mass source is 1 kg/sec at node No. 25 and the discharge is of the same value with negative sign at node No. 1. The initial concentration of the source element is 3 kg/m³ and the concentration value of 0 kg/m³ characterises other regular nodes. The retardation factor is specified as one.

The change of all constituents dissolved along the main transverse is illustrated in Fig. 4. The front of the maximal concentration is presented in Fig. 5.

The Figures show the processes accurately, namely the concentration decrease in versus of time in the system and its migration from the source to a sink node. The concentration values along the main transverse are listed in Table 1.

Number of node	Year	Concentration mg/l
25	0	3000
19	10	413
13	50	235
7	80	175
1	100	139

Version No. 2

Contamination with constant value in time is simulated and the movement of the concentration front is investigated.

Concentration of the regular nodes are zero, therefore the equilibrium is formed when the concentration equalises in each node over the system. Although this stable state did not occur during the simulation period of 190 years, the diagrams obtained show the trends properly.

The initial data are as follow:

- simulation time: 190 years
- printout time step: 10 years
- mass sink /water discharge/ at node No.1: -1 kg/s
- mass rate of contamination at node No. 25: 0.003 kg/s
- water recharge at node No. 25: 1 kg/s
- retardation factor 1

Change of concentration along the transverse is shown in Fig. 6.

Version No. 3

In this case the dilution was modelled. The initial concentration value of 3000 mg/l is valid for each regular node. The mass source is specified as "clear" water with zero concentration of all constituents dissolved. The seepage is induced by water recharge, which increases the pressure head of the system. The concentration changes occur both in the water flow value and in the increased water volume.

The initial data are as follow:

- simulation time: 100 years
- printout time step: 2 years
- water recharge at node No. 1: 1 kg/s
- concentration of each node: 3000 mg/l
- retardation factor: 1

The change of concentration along the main transverse is illustrated in Fig. 7.

CONCLUSIONS

As a result of a more extended research a numerical simulation model of solute transport was developed. The program code was prepared in Fortran IV /HWB 60/20/ and Microsoft 77 /IBM AT/ languages. The program is suitable to model complex seepage processes characterised by different conditions: as

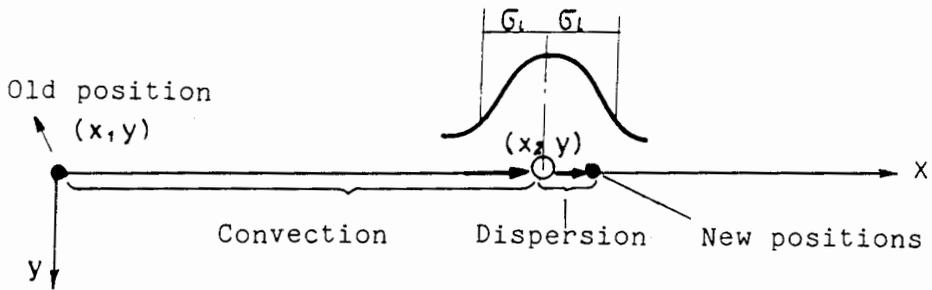
- two- or three-dimensional grid
- homogeneous or heterogeneous aquifer
- confined, unconfined or combined aquifer
- water recharge or discharge with constant or different rate in time

- interaction between surface waters and underground reservoirs
- injection of contaminated water
- leakage from waste disposed on the surface
- mixing the waters with different quality of aquifers
- thermal problems
- dispersion, dilution in waters and mixing of waters of different concentrations.

The neglect of the terms of the governing equations, which are unnecessary for the actual investigation, is very advantageous feature of the program code.

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New positions = Old positions + Convection + Dispersion

$$x_2, y = x_1, y + V_x \cdot \Delta t + \sqrt{2d_l \cdot V_x \Delta t} \cdot A(0)$$

where

V_x = Interstitial velocity of the groundwater in the x direction

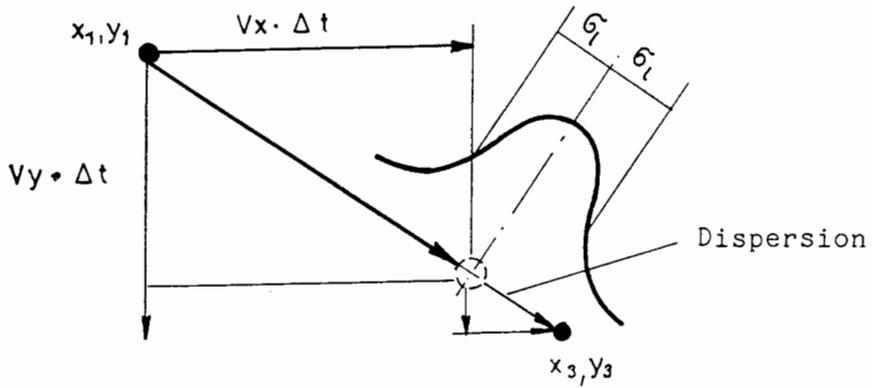
Δt = Time increment

d_l = Longitudinal dispersion

$A(0)$ = Random factor

Movement of a particle in case of longitudinal dispersion where the flow direction is aligned with x axis.

Figure 1.



New position = Old position + Convection + Dispersion

$$\begin{aligned} x_3 &= x_1 + V_x \Delta t + \sqrt{2d|V_x \Delta t|} \cdot A(0) \\ y_3 &= y_1 + V_y \Delta t + \sqrt{2d|V_y \Delta t|} \cdot A(0) \end{aligned}$$

Movement of a particle in case of longitudinal dispersion, where the flow direction is not aligned with x or y axis

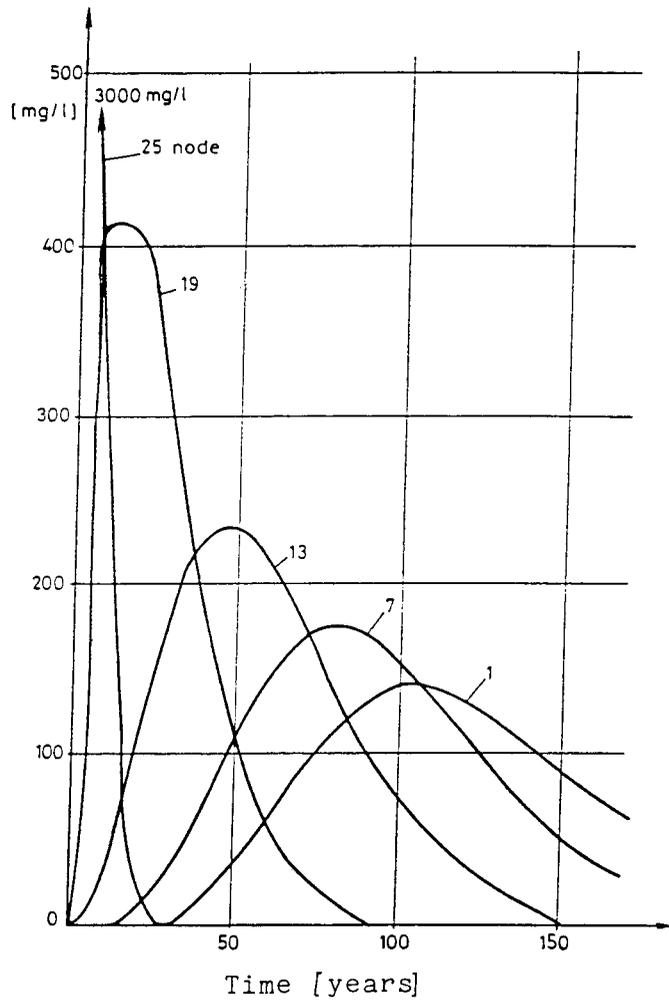
Figure 2.

5	10	15	20	25
4	9	14	19	24
3	8	13	18	23
2	7	12	17	22
1	6	11	16	21

Finite difference grid of the test model

Figure 3.

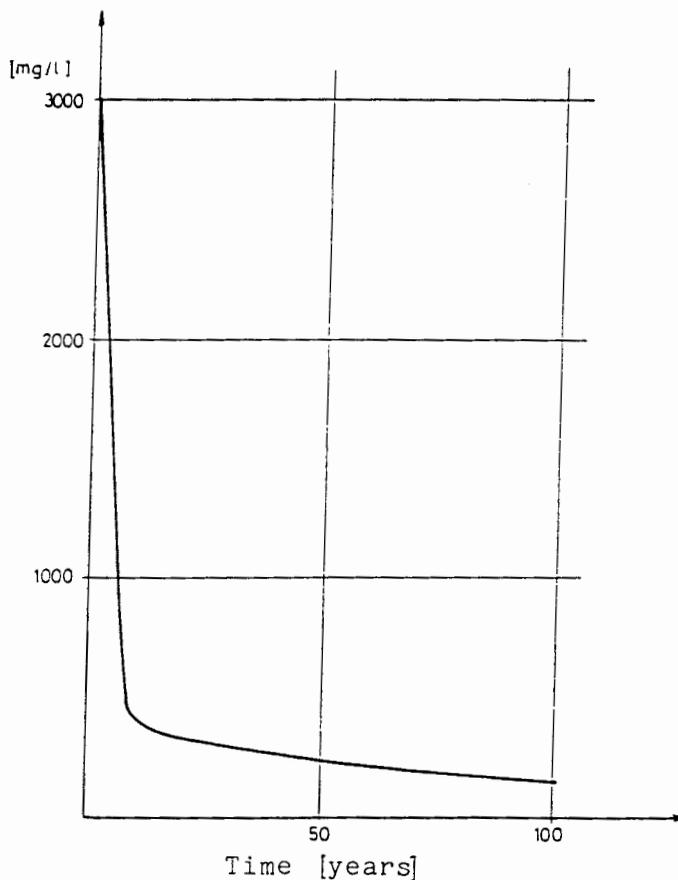
Concentration of
total dissolved solids



Variation of total dissolved solids along the main transverse in case of instantaneous feed of total solids

Figure 4.

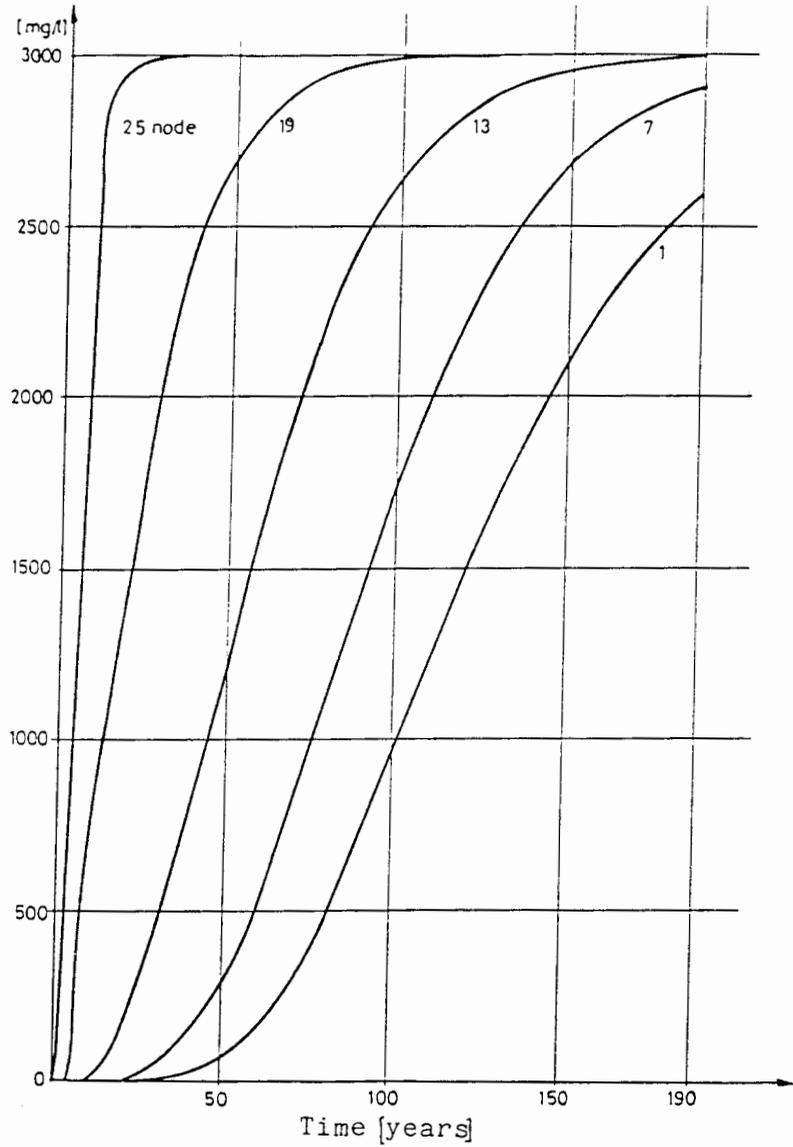
Concentration of
total dissolved
solids



Advance of the maximum of total dissolved solids, in case of instantaneous feed of total solids.

Figure 5.

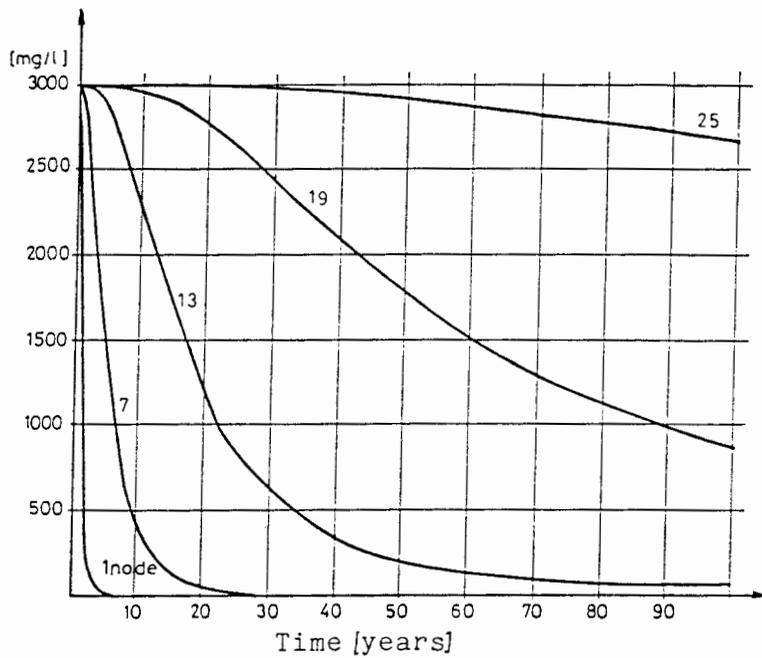
Concentration of
total dissolved
solids



Variation of total dissolved solids along the main transverse, in case of permanent feed of total solids

Figure 6.

Concentration of
total dissolved
solids



Variation of the concentration of total dissolved solids along the main transverse, in case of dilution. Source cell:No.1.

Figure 7.