Effect Of Soil Consistency On Flow Characteristics Of Acids Through Cohesive Soils

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Received on: 29/4/2007
Accepted on:3/4/2008

Abstract:
The consistency of cohesive soil depends to a large extent on the structure of soil particles which may be arranged in two systems; dispersed or flocculated. The presence of salts or acids between the soil particles will alter the arrangement of particles through affecting the attractive and repulsive forces.

In this paper, a program of laboratory tests is carried out at the University of Technology/ Baghdad on cohesive soils of different values of Atterberg limits. Samples of these soils were tested for grain size distribution (sieve analysis and hydrometer). The falling head permeability test was carried out to determine the coefficient of permeability of the soils to HCl acid.

The soil parameters determined in the laboratory will be used in the numerical analysis.The aim of this study is to apply the finite element method to study the steady flow of pollutants (acids) in a confined aquifer. The program (MULAT) is used for this purpose. The path of flow of the acid through the soil is traced.

The basic problem solved in this paper is a one of linear flow in a single confined aquifer. It represents the case of leakage of acids from storage tank and flow of the acids through the foundation soil. It was concluded from the finite element results that the maximum head caused by the flow of the acid through the soil decreases with the increase of the coefficient of permeability and the plasticity index of the polluted soil.

Key Words: Pollution, Cohesive soil, Acid, Finite elements.

تأثير قوام التربة على خصائص جريان الحوامض في الترب التماسكية

الخلاصة:
يعتمد قوام الترب التماسكية إلى حد كبير على ترتيب و بنية حبيبات التربة التي يمكن أن تترتب بنظامين: منتشر و متجمع. ان وجود الأملاح و الحوامض بين حبيبات التربة سوف يغير ترتيب الحبيبات من خلال التأثير على قوى التجاذب و التنافر.

في هذا البحث أجري برنامج فحوص مختبرية في الجامعة التكنولوجية ببغداد على ترب تماسكية ذات حدود أتربيرغ مختلفة، حيث فحصت نماذج من هذه الترب لتحديد توزيع أحجام الحبيبات (تحليل منخلي و تحليل المكثاف). و أجري فحص النفاذية (الشحنة الساقطة) لإيجاد معامل نفاذية هذه الترب لحامض الهيدروكلوريك Hcl . ان معاملات التربة التي تم إيجادها مختبريا سيتم استخدامها في التحليل العددي.

إن الهدف من هذه الدراسة هو تطبيق طريقة العناصر المحددة لدراسة الجريان الهادئ للملوثات (الحوامض) في حشرج محصور. و أستخدم برنامج الحاسبة المسمى (MULAT) لهذا الغرض. و تم تتبع مسار جريان الحامض خلال التربة. المسألة الأساسية التي تم حلها في هذا البحث هي مسألة جريان خطي في حشرج محصور منفرد و التي تمثل حالة نضوح لحوامض من خزان و جريان الحوامض خلال تربة

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https://doi.org/10.30684/ etj.26.10.4
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الأساس. و قد تم التوصل الى نتيجة من خلال طريقة العناصر المحددة مفادها أن الشحنة الكليـــة المتولـــدة نتيجة جريان الحامض خلال التربة تناقص مع زيادة معامل النفاذية و مؤشر اللدونة للترب الملوثة.

1. Transportation In Porous Media

The analysis of transport phenomena in porous media enables to study the behaviour of pollutants in groundwater. In this paper, a three-dimensional numerical model is developed, on the basis of the usual two-dimensional schematization of the groundwater flow. The flow model is used to describe and predict the pressure in the fluid, and the fluid velocity. These data are then considered as input parameters for a transport model, which incorporates advection, dispersion, and decay. This procedure is applicable if the variations of the concentration of the pollutant do not influence the flow of the fluid. This will be the case if the fluid density is practically not influenced by the pollution concentration.

The required input parameters in this paper are found in the laboratory. These include the permeability of the soil to Hcl acid.

For the analysis of groundwater flow, many powerful techniques are available, ranging from analytic solutions to numerical models. These models are widely available, including computer codes, and they have been tested and validated extensively. Their validity and applicability is generally accepted, even though it remains a formidable practical problem to collect sufficiently accurate data, such as soil properties and hydraulic boundary conditions, for the model predictions to be in agreement with physical reality. In the field of transport modeling several theoretical difficulties are hampering the applicability of the various models, especially numerical models, (Verruijt, 1995).

Basic Equations

Consider a saturated porous medium, in which the motion of the fluid is described by the velocity field v. Deformations of the porous medium are assumed to be so small that the porosity *n* can be considered to be constant in time. The concentration of a certain substance (a pollutant), which is being transported by the fluid, is denoted by *c*. This concentration is defined as the mass of the pollutant per unit volume of the fluid. Part of the pollutant may be adsorbed by the porous medium, and the pollutant may be subject to decay.

The balance of mass of the pollutant in the fluid requires that, (Verruijt, 1995):

$$n\frac{\partial c}{\partial t} = -\nabla.(nw) - Q - nG_f \qquad \ldots\ldots(1)$$

where w is the transport vector of the pollutant, expressed as a discharge of mass of the pollutant per unit area of the fluid,

Q is the transfer of mass to the porous medium by adsorption, and

G_f represents the decay of the substance in the fluid.

The flux w consists of advection and dispersion:

$$w = cv - D.\nabla c \qquad \ldots\ldots.(2)$$

The first term in this expression represents the transport by advection, which is governed by the fluid velocity v. The second term represents transport by dispersion (including diffusion), D being the dispersion tensor. This will be considered in more detail later.

The concentration of the pollutant in the porous medium is denoted by $c^{/}$. Its definition is the mass of the pollutant per unit volume of the material constituting the porous medium matrix (the soil particles). Transport by diffusion in the porous medium is disregarded. The balance of mass in the porous medium requires that:

$$(1-n)\frac{\partial c'}{\partial t} = Q-(1-n)G_s \quad \text{.......(3)}$$

in which G_s, represents the decay of the substance in the solid material.
The transfer function Q is, of course, the same as in eq. (1).

The velocity of the fluid in a porous medium is often so small that there is a continuous state of equilibrium between the concentrations of pollutant in the porous medium with the concentration in the fluid. The parameter governing the transfer of mass from the fluid to the solid is the Peclet number for diffusion in the solids,

$$P_s = \frac{vd}{D_s} \quad \text{......(4)}$$

where: v is the magnitude of the fluid velocity,
d is a representative particle diameter, and
D_s is the diffusivity of the pollutant in the solid material.

The order of magnitude of the particle diameter d is 10^{-4} m, and the order of magnitude of the diffusivity for most substances is 10^{-9} m^2/s. This means that the Peclet number Ps is small compared to 1, provided that the velocity is small compared to 10^{-5} m/s, which is about 1 m/d. This may often be the case; in other cases it can still be assumed, as a first approximation that the concentrations are in equilibrium, (Verruijt, 1995).

It is now assumed that in the state of equilibrium the concentration of pollutant in the solids is proportional to the concentration in the fluid,

$$c' = Kc \quad \text{.......(5)}$$

in which K is a given constant.

This relation is usually called the *linear equilibrium isotherm.* For the transport of heat in a porous medium, equilibrium is usually considered to require that the temperatures of the fluid and the particles are equal. In that case K = 1. For the transport of a pollutant, equilibrium may be a consequence of various adsorptive processes. Some substances are attracted more by the solid particles than others. Thus the value of the *partitioning coefficient* K is dependent on the physical properties of the pollutant, the fluid and the porous material. For salt, the value of the partitioning coefficient K is very small: salt is practically not adsorbed by the soil.

With eq. (5), equation (3) may be written as:

$$Q = (1-n)K\frac{\partial c}{\partial t} + (1-n)G_s \quad \text{.........(6)}$$

Substitution of eq. (6) into eq. (1) gives:

$$R.n\frac{\partial c}{\partial t} = -\nabla .(n.w) - n.G_s \quad \text{.......(7)}$$

where: $nG = nG_f + (1 - n)G_s$, the total decay of the pollutant, and R is the retardation factor,

$$R = 1 + \frac{1-n}{n}K \quad \text{……(8)}$$

The retardation factor R is equal to 1 if the solid particles do not adsorb any fraction of the pollutant (K = 0). For a substance which in its equilibrium state is distributed homogeneously over the fluid and the solids, such as the temperature in a heat transport process, K = 1, and therefore R = 1/n. eq. (7) is the basic balance equation.

The velocity vector w in eq. (7) consists of an advective flux and a dispersive flux, as expressed by eq. (2),

$$w = cv - D.\nabla c \quad \text{……...(9)}$$

The first term in the right hand side represents the advective transport, which is the transport of the pollutant as if the particles are attached to the water particles. In many cases this is the main component of transport, and it is considered essential that this form of transport is described accurately in a model. The dispersive transport is described by a second order tensor D. The components of this tensor can be related to the velocity components as follows (Bear and Verruijt, 1987):

$$D_{ij} = Dd_{ij} + a_{ijkl} v_k v_l / v \quad \text{……(10)}$$

Here D is the coefficient of molecular diffusion (of the pollutant in the fluid),

δ_{ij} is the Kronecker delta ($\delta_{ji} = 1$, if i = j, and $\delta_{ji} = 0$, if $i \neq j$),

v_k indicates the component of the fluid velocity in the direction x_k, and

v is the magnitude of the fluid velocity.

$$v = \sqrt{v_k v_l} \quad \text{…….(11)}$$

3. Finite Element Solution

For the solution of groundwater flow problems, finite element models are widely used, and generally considered as a useful and powerful tool. This suggests to investigate the possibility to base a transport model on a finite element model. Such a model is presented below, in the program MULAT. The program applies to steady flow in a single confined aquifer, with the possibility of water supply from the exterior by a given infiltration in the elements, or by given discharges in the nodes (local wells). The program calculates the advective transport of a given number of particles, with given starting points, and traces the stream lines of these particles on the screen. An eventual retardation is not taken into account, although this can easily be simulated by a change of the time scale.

4. Three-Dimensional Transport

For the analysis of transport of pollutants in aquifers, it is often necessary to take into account the vertical component of flow, in order to obtain a realistic evaluation of the extent of the endangered zones. This can, of course, be accomplished by using a fully three-dimensional model, but this will lead to systems with many millions of degrees of freedom, requiring large computers and long computation times. Moreover, the usual geological geometry is such that the vertical dimensions are much smaller than the horizontal dimensions. This suggests using a mixed type of approach, in which the soil is considered to consist of a layered system of a number of aquifers, with interjacent layers of low permeability (aquitards).

In the sandy aquifers, the flow will be mainly horizontal, so that it can be assumed that the pressure distribution is hydrostatic (Dupuit's assumption). In the aquitards (usually clay layers) the flow can be considered to be strictly vertical. These layers serve to transfer water from one aquifer to another. In the aquifers, the flow velocity is considered fully three dimensional, with the vertical component of flow being determined from the equation of continuity (Strack, 1984). In this paper, this approach will be presented for a finite element analysis in a single layer.

A finite element analysis for a multi-layered system has been described by Verruijt and Swidzinsky (1993). The finite element analysis of the distribution of the groundwater heads in a single aquifer and this has been extended to the tracing of two-dimensional stream lines, in the program. This will lead to a solution in which the groundwater head f is a function of the coordinates x and y in the horizontal plane. The components of the specific discharge vector in the horizontal plane can be determined by using Darcy's law,

$$q_x = -k\frac{\partial f}{\partial x} \qquad \text{.......(12)}$$

$$q_y = -k\frac{\partial f}{\partial y} \qquad \text{.......(13)}$$

These will be functions of x and y. In particular, in a finite element model using triangular elements with linear interpolation of the head f, and a constant permeability in each element, the two components q_x and q_y will be constant in each element, but different in different elements.

If the vertical component of flow q_z now would also be derived from Darcy's law the result would be zero, because the derivative $\partial f/\partial z$ is zero.

Therefore it is suggested, following Strack (1984), that this component be determined from the equation of continuity of an element in the aquifer,

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = 0 \qquad \text{..................(14)}$$

It now follows that:

$$\frac{\partial q_z}{\partial z} = -\frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} = A(x, y) \qquad \text{..........(15)}$$

where the function A(x, y) indicates that the right hand side of the equation is independent of z.

Integration of equation (15) in z - direction now gives:

$$q_s = A(x, y)z + B(x, y) \qquad \text{...............(16)}$$

where B(x, y) is an integration constant, again a function of x and y only.

The two functions *A* and *B* can be determined most simply from the boundary conditions in vertical direction. First of all, it is assumed here that the bottom of the aquifer is horizontal, and completely impermeable If the level of this bottom is denoted as the surface z = 0 it follows that the first boundary condition is:

$$z=0 : q_z = 0 \quad \text{....(17)}$$

This gives, with eq. (16),

$$B = 0 \quad \text{.....(18)}$$

For a steady free surface, the boundary condition at the upper surface is (Verruijt, 1995)

$$z = f : \quad q_z - q_x \frac{\partial f}{\partial x} - q_y \frac{\partial f}{\partial y} + I = 0 \quad \text{......(19)}$$

where I is the infiltration rate. This condition ensures that the infiltration is added to the system. It also ensures that the free surface is a stream line boundary when there is no infiltration.

Because the derivatives $\partial f/\partial x$ and $\partial f/\partial y$ can be expressed into the fluxes q_x and q_y using Darcy's law, as in eqs. (12) and (13), the boundary condition (19) can also be written as, (Verruijt, 1995):

$$z = f : \quad q_z = -I - \frac{q_x^2 + q_y^2}{k} \quad \text{........(20)}$$

With equation (16) the value of the function A can now be determined:

$$A = -\frac{I}{f} - \frac{q_x^2 + q_y^2}{kf} \quad \text{......(21)}$$

The final expression for the vertical component of the specific discharge is:

$$q_z = -(I - \frac{q_x^2 + q_y^2}{k})\frac{z}{f} \quad \text{.............(22)}$$

All components of the flow now are completely known. It appears that the vertical component is a linear function of *z*. This is a consequence of Dupuit's assumption. It has been shown that this approximation is very good, provided that the vertical dimension of the system is indeed small compared to the horizontal dimensions (Strack, 1989 and Verruijt, 1991). It should be noted that the velocity components can be determined from the specific discharge by dividing them by the effective porosity *n*.

5. Testing Program

A series of tests were carried out to investigate the relationship between the consistency of cohesive soil described by its plasticity index and the coefficient of permeability. Four samples of clays were selected and the following tests were incorporated:

1. Grain size distribution including:
   a) Sieve analysis according to ASTM-D422 specifications.
   b) Hydrometer analysis according to ASTM-D422 specifications.
2. Liquid and plastic limits according to ASTM-4318 specifications.

3. Falling head permeability test to investigate the permeability of the clayey soils to Hcl acid instead of water.

Fig. (1) shows the grain size distribution for the four samples while Fig. (2) presents the relationship between the plasticity index and coefficient of permeability of the clays to Hcl acid. Fig. (3) shows the variation of the coefficient of permeability to Hcl acid with the percent of clays. All samples were remolded to have a constant dry unit weight of (15 kN/m^3) and a water content of 20%.

6. Computer Program

MULAT is a program for the analysis of steady plane groundwater flow in a system of aquifers, separated by aquitards, using the finite element method, with triangular elements. The program calculates the groundwater head in the layers, under the influence of boundary conditions, infiltration (rain) on the upper surface, and local pumping wells. The program will show the groundwater head in the form of contours, or as a surface in three-dimensional space. The program can also show the pathlines of particles, as they are transported by the groundwater. The flow in the aquifers is assumed to be mainly horizontal, with the groundwater head being independent of the vertical coordinate. The vertical velocity in the aquifers is calculated from the continuity equation. In the aquitards the flow is strictly vertical. The program was written in C++, using Borland's C++Builder and later made a software.

Each layer of the system is subdivided into a large number of small triangles : the finite elements. In each layer the same mesh of finite elements is used. The mesh is generated on the basis of a relatively small number of triangular blocks. All soil properties (such as the permeability k) are constant in each block. The thickness of each layer is defined by specifying the elevation of the bottom (B) of the aquifer and the elevation of its top (T) in the three nodes constituting a block (these are called the main nodes). In all interior points the thickness of the layer is interpolated linearly between the values in the three main nodes. The transmissivity (TR) of each layer is defined as the product of permeability and thickness : TR=k*(TB) if the groundwater head (F) is above the top of the aquifer. If the groundwater level is below the top of the aquifer the transmissvitiy is defined as TR=k*(FB). This means that the aquifer is confined when the groundwater level is above the top of the aquifer, and unconfined when the groundwater level is below the top of the aquifer. The elevation of the bottom of the deepest layer can not be below 0 m.

The solution procedure is iterative, with cycles and iterations. In is estimated on the basis of the results of the previous cycle, with TR=k*(FB). In the first cycle TR=k*(TB), independent of the value of F. The number until the total unbalance in the water balance is very small.

7. Modeling The Problem

The basic problem is a one of linear flow in a single confined aquifer. It represents the case of leakage of acids from storage tank and flow of the acids through the foundation soil. The length of the region is 2000 m, its width is 2000 m, the aquifer thickness is 9 m, the permeability is for the first sample is measured to be $84x10^{-6}$ 10 m/day (as shown in Figure 3 for sample 3), the porosity is 0.44, and the retardation factor is 1. The lower boundary in the plane of flow is impermeable. In this case the solution is that the groundwater head varies linearly, from 9 m to 0 m. The hydraulic gradient is 0.0045, and the specific discharge is, with Darcy's law, 3.78×10^{-6} m^3/day. Because the porosity is 0.4 and the retardation factor is 1, it follows that the velocity of the particles is 0.125 m/d. The time interval between marks is set to 200 days, so that the distance traveled by a particle between two marks is 125 m. When running the program, and inspecting the path lines of the particles, it is found that marks are set at mutual distances of 125 m, indicating that the velocities are calculated correctly by the program.

The input parameters for the basic problem are given in Table (1). The finite element mesh is drawn in Fig. (4).

8. Finite Element Results

The results may well be useful as a first indication of the general trend of the transport process, however. Figures (5) to (8) show the contour lines through the soil below the pollted area. Figure (9) shows the relationship between the permeability of the soil to the acid and the maximum head caused by the flow of the polluting acid. Figure (10) shows a similar relationship between the plasticity index and the head. It can be noticed that the maximum head caused by the flow of the acid through the soil decreases with the increase of the coefficient of permeability and the plasticity index of the polluted soil.

9. Conclusions

A three-dimensional numerical model is developed on the basis of the usual two-dimensional schematization of the groundwater flow. The flow model is used to describe and predict the pressure in the fluid, and the fluid velocity. The finite element method is used in the analysis.

The basic problem solved in this paper is a one of linear flow in a single confined aquifer. It represents the case of leakage of acids from storage tank and flow of the acids through the foundation soil. The soil parameters required for the finite element model were determined in the laboratory. These include the coefficient of permeability of the soil to Hcl acid. It was concluded from the finite element results that the maximum head caused by the flow of the acid through the soil decreases with the increase of the coefficient of permeability and the plasticity index of the polluted soil.

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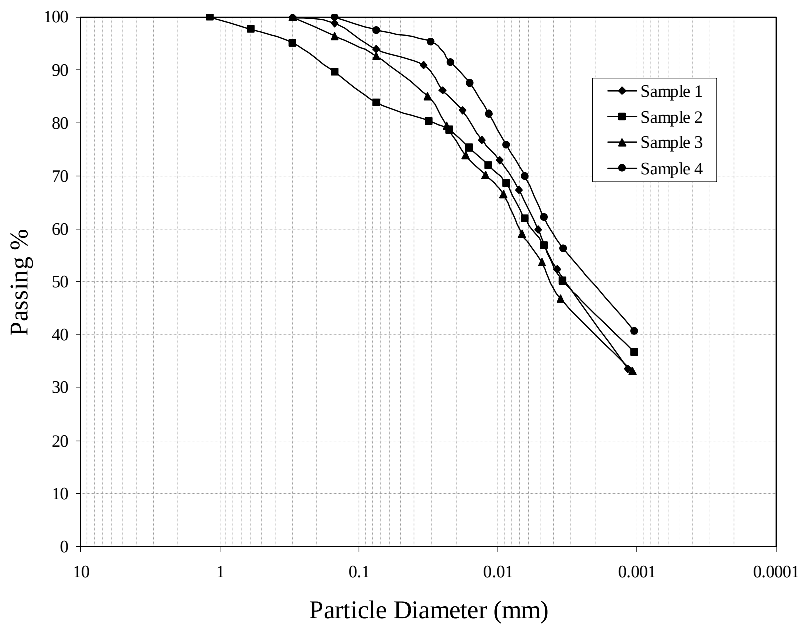


Fig. 1 The grain size distribution for the selected samples.

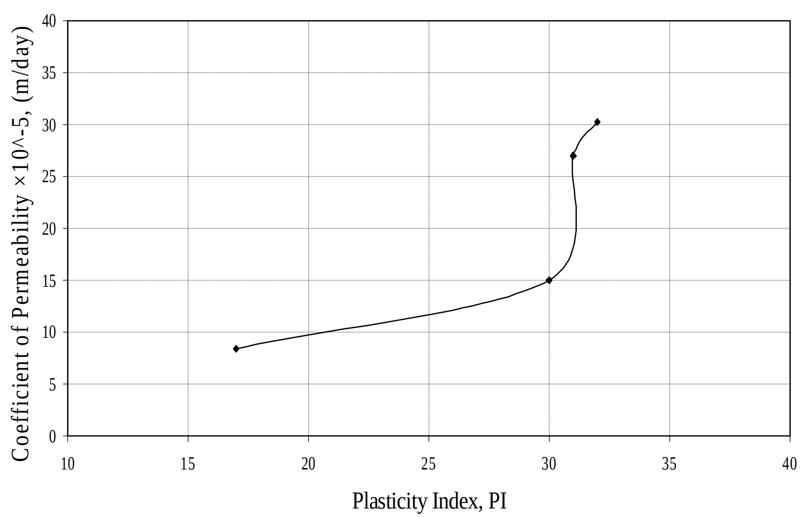
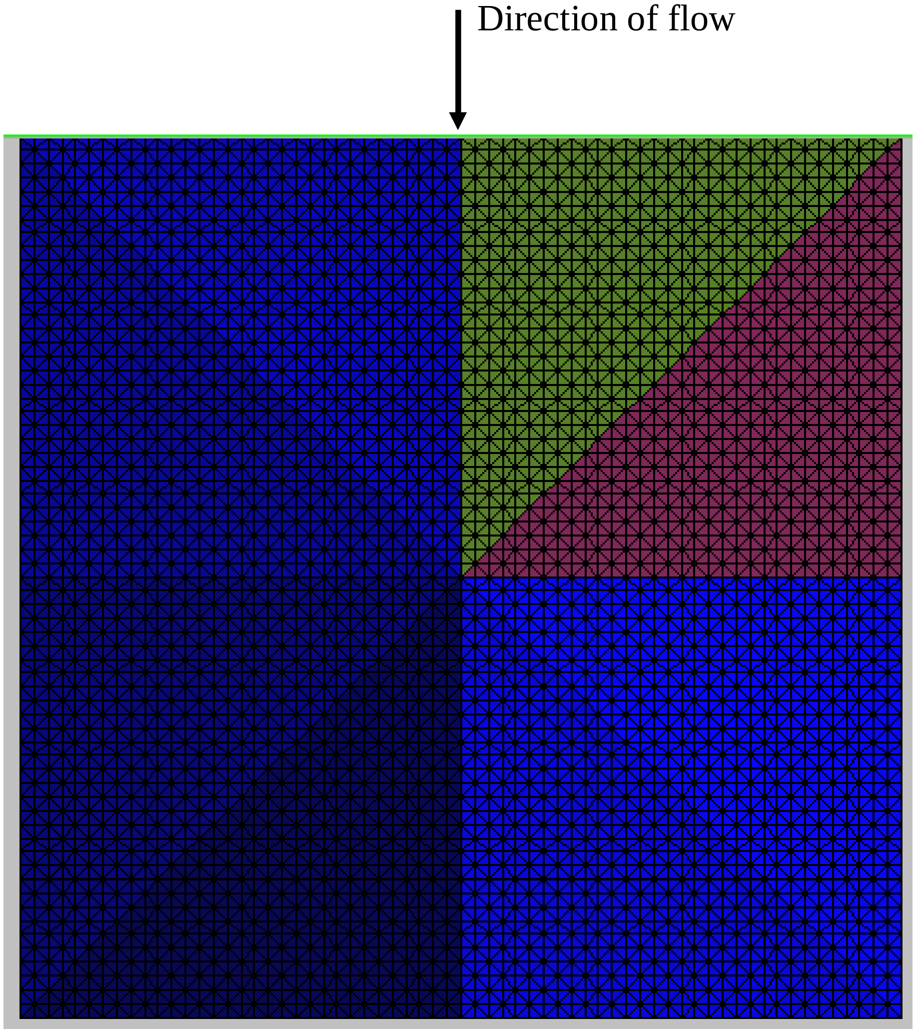


Fig. 2 The relation between the coefficient of permeability and the plasticity index.

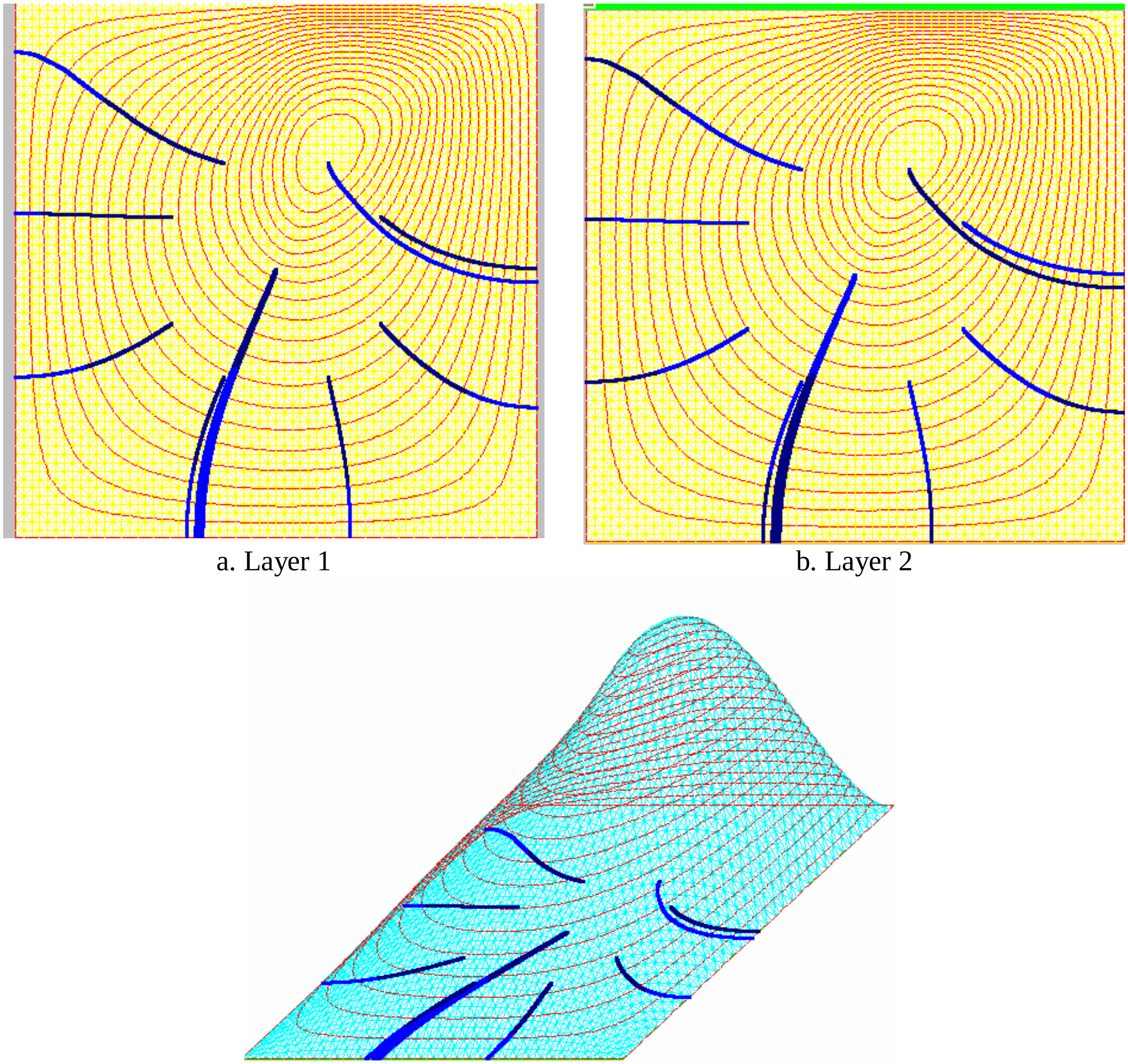
Fig. 3 The relation between the coefficient of permeability and the percent of clay particles.



Impermeable boundary

No. of elements = 8192. No. of nodes = 4225.

Fig. 4. The finite element mesh.

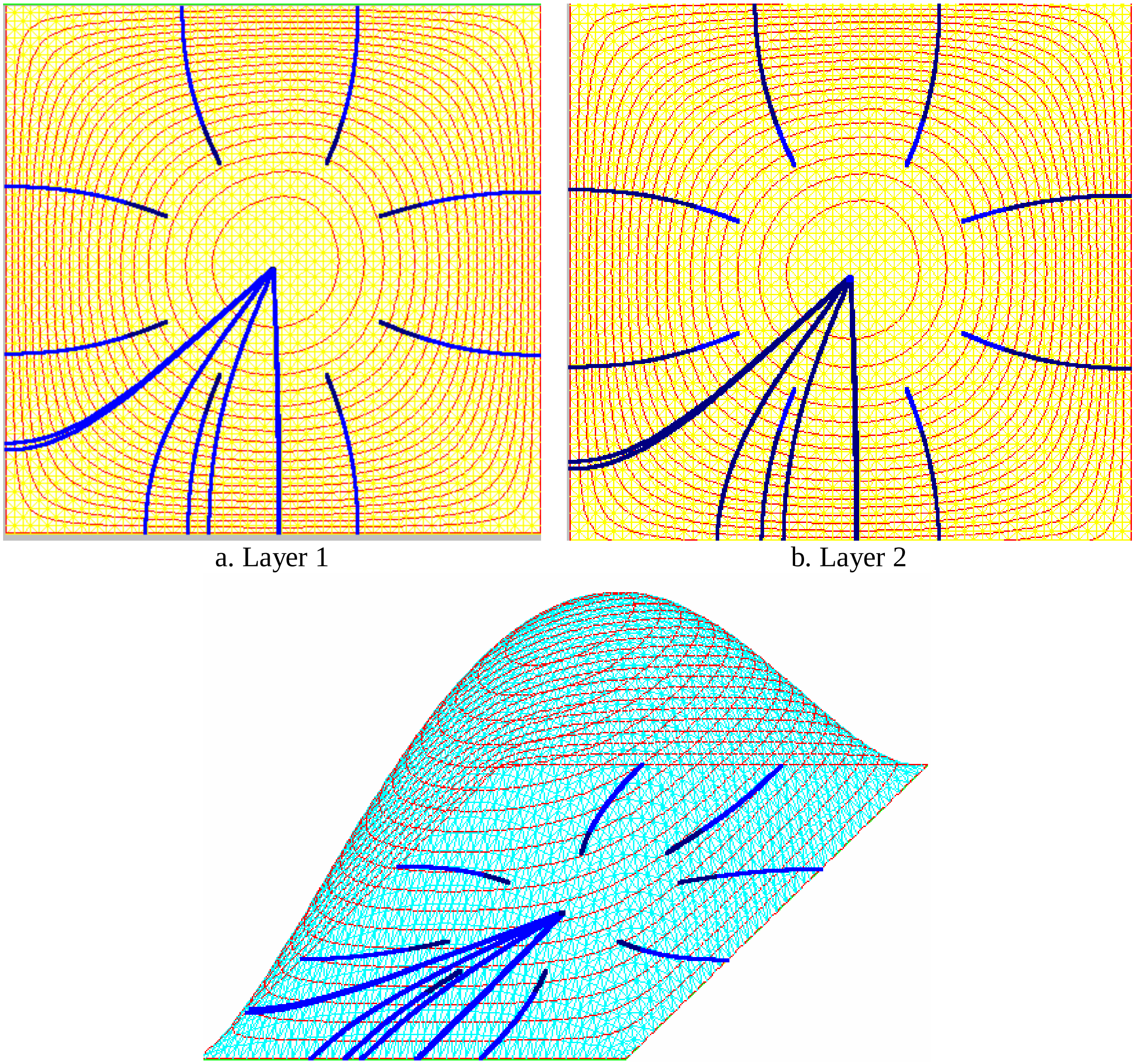


a. Layer 1

b. Layer 2

c. Three-dimensional distribution.

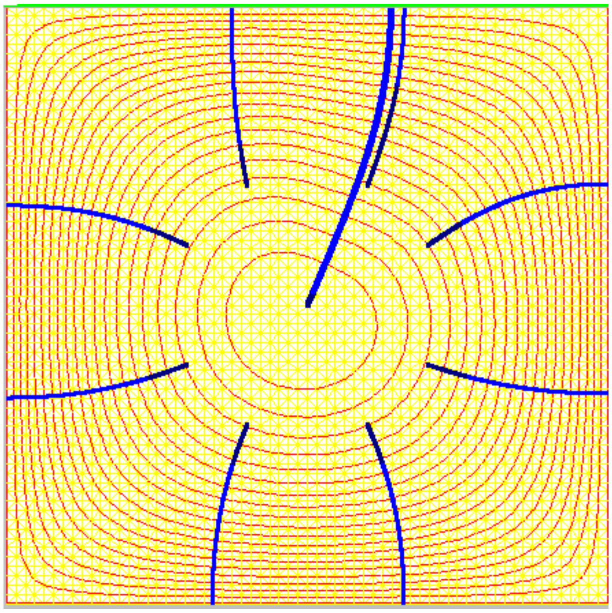
Fig. 5 Contour lines of heads below the polluted area (k_f = 84x10^{-6} m/day).
Note: Maximum contour: 45720 mm, minimum contour: 20 mm, contour interval: 2285 mm.



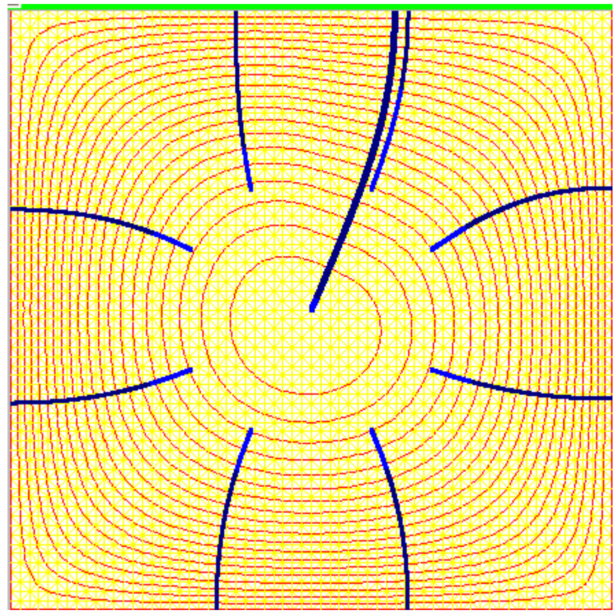
a. Layer 1 b. Layer 2

c. Three-dimensional distribution.

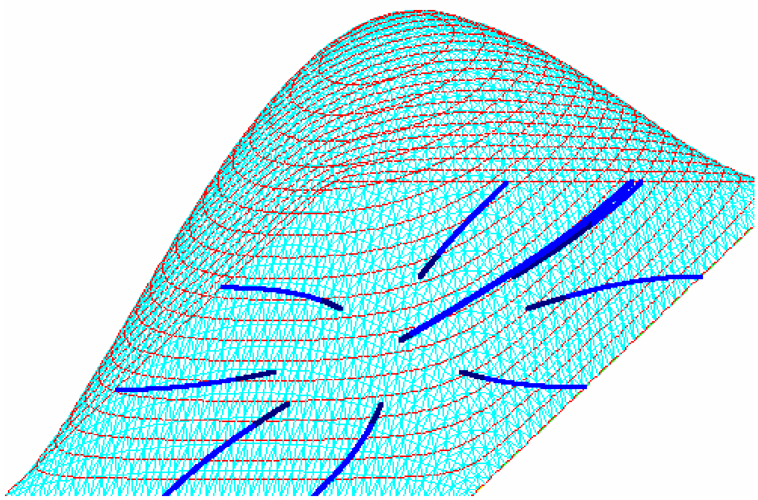
Fig. 6 Contour lines of heads below the polluted area (k_f = 15.5x10^{-5} m/day).
Note: Maximum contour: 15914 mm, minimum contour: 20 mm, contour interval: 794.7mm.



a. Layer 1

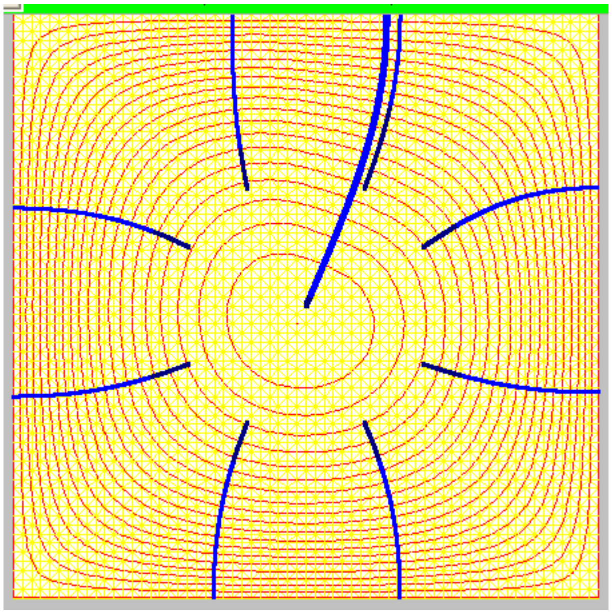


b. Layer 2

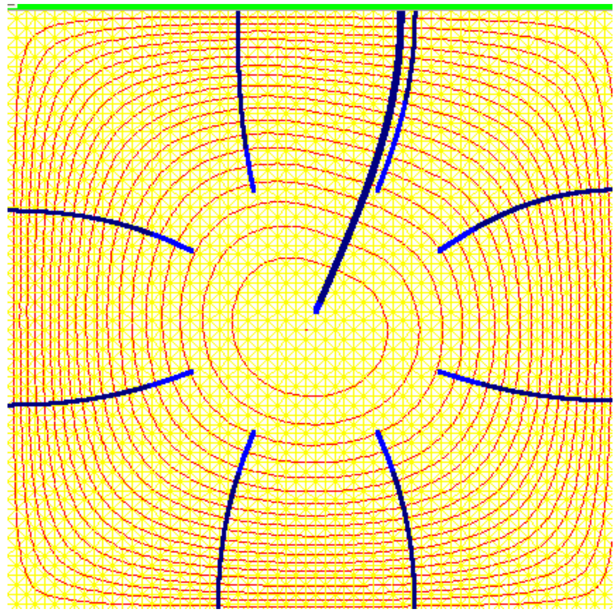


c. Three-dimensional distribution.

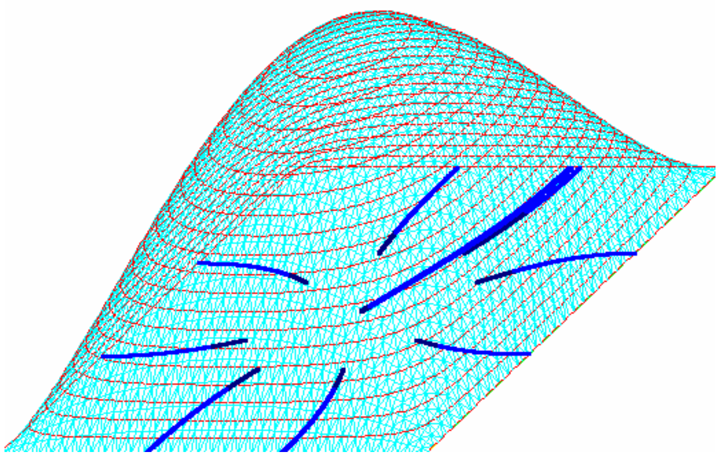
Fig. 7 Contour lines of heads below the polluted area ($k_f = 30x10^{-5}$ m/day).
Note: Maximum contour: 13930 mm, minimum contour: 20 mm, contour interval: 732.1mm.



a. Layer 1



b. Layer 2



c. Three-dimensional distribution.

Fig. 8 Contour lines of heads below the polluted area (k_f = 27x10^{-5} m/day).
Note: Maximum contour: 14666 mm, minimum contour: 20 mm, contour interval: 723.3 mm.

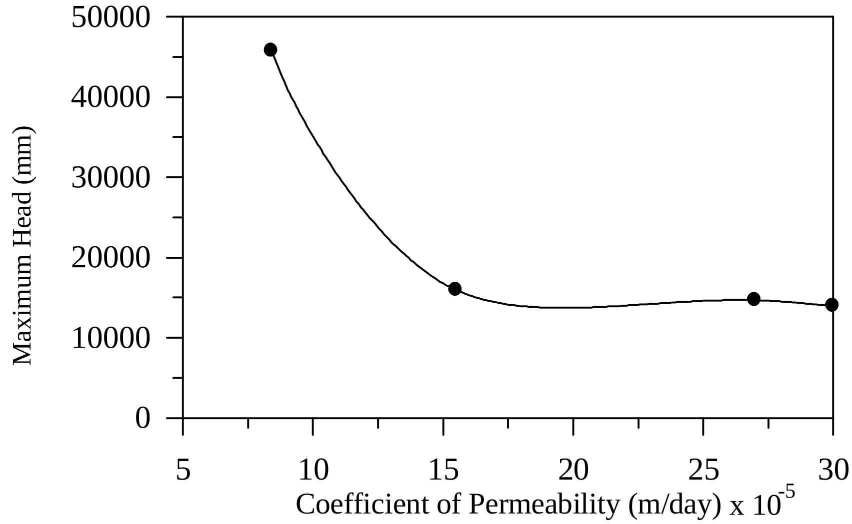


Fig. 9 Variation of the maximum head in the region with the coefficient of permeability of the soil to acid.

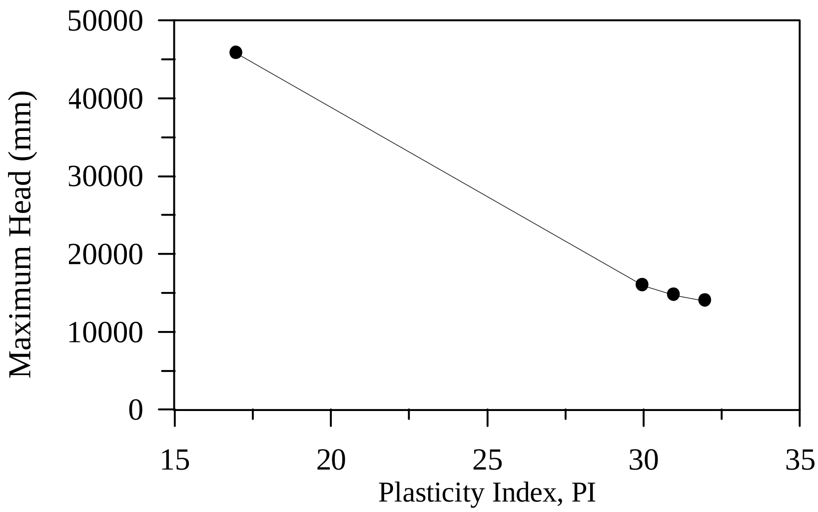


Fig. 10 Variation of the maximum head in the region with the plasticity index of the soil.