

FINITE ELEMENT METHODS IN HYDROGEOLOGY

by

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RESUME

Ce rapport présente les notes de cours prises lors du Séminaire sur l'emploi de la Méthode des Eléments Finis en Hydrogéologie, qui s'est tenu à Orléans-La Source du 4 au 15 septembre 1972, organisé conjointement par le BRGM, l'Ecole des Mines de Paris et le Volcani Center (Israël).

L'enseignement a été donné en anglais par :

- . le Professeur P.A. WITHERSPOON, Professeur de Géologie de l'Ingénieur à l'Université de Californie,
- . et par le Docteur S.P. NEUMAN, Senior Scientist au Volcani Center d'Israël.

Le texte, constitué de notes directement rédigées en langue anglaise pendant les cours du séminaire n'a pas encore été revu par les conférenciers, et nous présentons nos excuses pour les erreurs qui peuvent s'y trouver. Nous remercions d'avance les lecteurs pour les remarques et corrections qu'ils pourraient nous signaler.

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Introduction

This document is a first draft of notes taken during the SEMINARS ON FINITE ELEMENT METHODS IN HYDROGEOLOGY, which were held in Orleans from September 4th to September 15th 1972. It has been directly written in English during the lectures delivered by Pr. P.A. WITHERSPOON (University of California) and Dr. S.P. NEUMAN (Volcani Center).

This copy has not yet been corrected by the lecturers and we apologize for the errors that might be encountered. Any remark and correction will be gladly met.

The completion of this paper needed a lot of work for which we are much indebted to Mr. G. ASSENS, J.-L. DESSENNE, E. LEDOUX, G. de MARSILY and M. VANDENBEUSCH.

We especially acknowledge the work of Mrs. G. PAQUIN who typed very efficiently the manuscript with so many mathematic symbols.

A corrected version of this document translated into French will be issued next Spring in "Bulletin du Bureau de Recherches Géologiques et Minières".

J.-P. SAUTY

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INTRODUCTION : DEFINITION OF THE PROBLEM

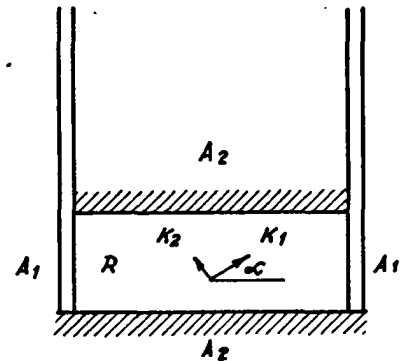
The problem of groundwater flow in a region R is to determine the head h and the velocity v_i at any point x_i in R, given

- boundary conditions, which may be of 2 types
 - . prescribed head on A_1
 - . prescribed flux on A_2
- permeability in R, which may be heterogeneous and anisotropic, with different anisotropies in each point.

In 2 dimensions, this permeability is represented by a tensor, noted

$$K_{ij} = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}$$

- storage coefficient, S_s or S_y
- thickness of aquifer in the case of horizontal plane flow
- pumpage from wells
- areal recharge or discharge.



EQUATIONS : in steady state

equation of continuity	$\frac{\partial v_i}{\partial x_i} = 0$	}	on R	(1)
Darcy's law	$v_i = - K_{ij} \frac{\partial h}{\partial x_j}$	}	on R	(2)
Prescribed head on A_1	$h(x_i) = H(x_i)$		on A_1	(3)
Prescribed flux on A_2	$v_i(x_i) \cdot n_i(x_i) = V(x_i)$		on A_2	(4)

Equations (1) + (2) give

$$\frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j} \right) = 0 \quad \text{on } R \quad (5)$$

h and v_i are unknown functions defined on R

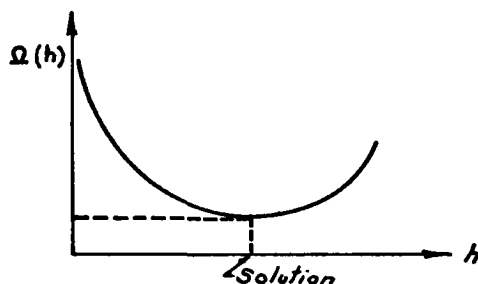
Repeated indices indicate summation over $i, j = 1, 2, 3$.

VARIATIONAL PRINCIPLES

A functional Ω of a function h is a real number $\Omega(h)$ associated with any function h defined on the region R .

Different functions h_1 and h_2 defined on R will give generally different numbers $\Omega(h_1)$ and $\Omega(h_2)$. If an appropriate functional Ω is defined for the problem stated by equations (1) to (5), the unique solution h of the problem of flow in R is the one that minimizes the value of $\Omega(h)$.

In a schematic representation :



FUNCTIONAL FOR STEADY STATE

It is, in terms of head :

$$\Omega(h) = \int_R \frac{1}{2} K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial h}{\partial x_i} dR - \int_{A_1} (h - H) K_{ij} \frac{\partial h}{\partial x_j} n_i dA + \int_{A_2} V h dA$$

We will see later how this can be derived.

Those integrals are definite integrals.

PRINCIPLE OF FIRST VARIATION

The first variation of $\Omega(h)$ is defined by :

$$\delta\Omega(h) \equiv \frac{d}{d\lambda} \left[\Omega(h + \lambda\tilde{h}) \right]_{\lambda=0}$$

where \tilde{h} is any admissible function satisfying

$$\begin{cases} \tilde{h} = 0 & \text{on } A_1 \\ \frac{\partial\tilde{h}}{\partial n} = 0 & \text{on } A_2 \end{cases}$$

where n is the normal at A_2 .

Property : the functional $\Omega(h)$ is appropriate to solve the problem if and only if $\delta\Omega(h) = 0$.

VERIFICATION OF THE VALIDITY OF THE GIVEN FUNCTIONAL FOR STEADY STATE

Let us apply the principle of first variation

$$\delta\Omega(h) = \frac{d}{d\lambda} \left[\int_R \frac{1}{2} K_{ij} \frac{\partial(h + \lambda\tilde{h})}{\partial x_j} \frac{\partial(h + \lambda\tilde{h})}{\partial x_i} dR - \int_{A_1} (h + \lambda\tilde{h} - H) K_{ij} \frac{\partial(h + \lambda\tilde{h})}{\partial x_j} n_i dA + \int_{A_2} V(h + \lambda\tilde{h}) dA \right]_{\lambda=0}$$

Since $K_{ij} = K_{ji}$,

$$\delta\Omega(h) = \int_R K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial\tilde{h}}{\partial x_i} dR - \int_{A_1} \left[(h-H) K_{ij} \frac{\partial\tilde{h}}{\partial x_j} + \tilde{h} K_{ij} \frac{\partial h}{\partial x_j} \right] n_i dA + \int_{A_2} V\tilde{h} dA$$

Let us apply Green's first identity to the functions $K_{ij} \frac{\partial h}{\partial x_j}$ and \tilde{h} ; we can write :

$$\int_R \left[\tilde{h} \frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j} \right) + K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial \tilde{h}}{\partial x_i} \right] dR \equiv \int_{A_1} \left(\tilde{h} K_{ij} \frac{\partial h}{\partial x_j} \right) n_i dA + \int_{A_2} \left(\tilde{h} K_{ij} \frac{\partial h}{\partial x_j} \right) n_i dA$$

Substituting this identity in $\delta\Omega(h)$ and after some manipulations we obtain :

$$\delta\Omega(h) = - \int_R \underbrace{\tilde{h} \frac{\partial}{\partial x_i} K_{ij} \frac{\partial h}{\partial x_j}}_{\alpha} dR - \int_{A_1} \underbrace{(h-H) K_{ij} \frac{\partial \tilde{h}}{\partial x_j} n_i}_{\beta} dA + \int_{A_2} \underbrace{\left(K_{ij} \frac{\partial h}{\partial x_j} n_i + V \right)}_{\gamma} \tilde{h} dA$$

For arbitrary \tilde{h} , this is equal to zero if and only if $\alpha \equiv \beta \equiv \gamma = 0$. Then, $\Omega(h)$ is an appropriate functional for the resolution of our problem described by equation (1) to (5).

SUFFICIENT CONDITION

If $\delta\Omega(h) = 0 \forall \tilde{h}$, \tilde{h} must vanish : so the terms α , β and γ are all equal to zero. These terms represent the governing equation (5) in R , and the boundary conditions (3) and (4) which are then satisfied.

NECESSARY CONDITION

If equations (3), (4) and (5) are satisfied, the corresponding integrals are equal to zero and then $\delta\Omega(h) = 0$. The given functional $\Omega(h)$ is consequently an appropriate one, and the solution h of our problem is the function that minimises $\Omega(h)$.

ANOTHER FUNCTIONAL FOR STEADY STATE

If we want solutions in terms of head and velocity simultaneously, another functional must be defined. For instance, the study of dispersion leads to use a functional in terms of h and v_i :

$$\Omega(h, v_i) = \int_R \left[v_i \frac{\partial h}{\partial x_i} + \frac{1}{2} v_i K_{ik}^{-1} v_k \right] dR - \int_{A_1} (h-H) v_i n_i dA + \int_{A_2} V h dA$$

this functional gives a solution to equation (1) to (4). It is possible with it to have a better approximation of the velocity than ^{the one we obtain by} just using equation (2) when the head is known (less discontinuity). In this case, the solution of the problem can be shown to be given by the scalar function h and the vector function v_i that minimise simultaneously the value of Ω .

FUNCTIONAL FOR NON-STEADY STATE

S_s will be the specific storage. The equation of continuity becomes

$$\frac{\partial v_i}{\partial x_i} = - S_s \frac{\partial h}{\partial t} \quad \text{on } R \quad (6)$$

associated with Darcy's law (2) it gives

$$\frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j} \right) = S_s \frac{\partial h}{\partial t} \quad \text{on } R \quad (7)$$

Boundary conditions are defined again by equation (3) and (4). It is necessary to give initial conditions

$$h(x_i) = h_0 \quad \text{on } R \quad (8)$$

Using GURTIN's approach, it is possible to introduce the initial conditions (8) into equation (6).

Let us apply the Laplace transform to equation (6), using equation (8) and noting \bar{x} the Laplace transform of x :

$$\bar{x} = \int_0^{\infty} e^{-Pt} x dt$$

$$\overline{\frac{\partial v_i}{\partial x_i}} = -S_s \overline{\frac{\partial h}{\partial t}} = -S_s \int_0^{\infty} e^{-pt} \frac{\partial h}{\partial t} dt = -S_s \left\{ \left[h e^{-pt} \right]_0^{\infty} + p \int_0^{\infty} h e^{-pt} dt \right\}$$

$$\overline{\frac{\partial v_i}{\partial x_i}} = -S_s (p\bar{h} - h_0)$$

$$\frac{1}{p} \overline{\frac{\partial v_i}{\partial x_i}} = -S_s \left(\bar{h} - \frac{h_0}{p} \right)$$

Using the following property of Laplace transform :

$$\overline{x \cdot y} = \int_0^t x(z)y(t-z) dz = \overline{(x*y)} \quad (* = \text{convolution})$$

and coming back to the real functions we obtain

$$1 * \frac{\partial v_i}{\partial x_i} = -S_s (h - h_0) \quad \text{which combines equation (6) + (8)}$$

Our system of equations can now be written

$$\left\{ \begin{array}{l} 1 * \frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j} \right) = S_s (h - h_0) \quad \text{on } R \\ h = H \quad \text{on } A_1 \\ K_{ij} \frac{\partial h}{\partial x_j} n_i = -V \quad \text{on } A_2 \end{array} \right.$$

An appropriate functional is :

$$\begin{aligned} \Omega(h) = & \int_R \left[\frac{1}{2} * K_{ij} \frac{\partial h}{\partial x_j} * \frac{\partial h}{\partial x_i} + S_s \left(\frac{1}{2} h * h - h * h_0 \right) \right] dR \\ & - \int_{A_1} 1 * (h-H) * K_{ij} \frac{\partial h}{\partial x_j} n_i dA + \int_{A_2} 1 * V * h dA \end{aligned}$$

We can also calculate the first variation of this functional, using Green's first identity :

$$\begin{aligned} \delta\Omega(h) = & \int_R \left[-1 * \frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j} \right) + S_s (h - h_0) \right] * \tilde{h} \, dR \\ & - \int_{A_1} 1 * [h-H] * K_{ij} \frac{\partial \tilde{h}}{\partial x_j} n_i \, dA + \int_{A_2} 1 * \left[K_{ij} \frac{\partial h}{\partial x_j} n_i + V \right] * \tilde{h} \, dA \end{aligned}$$

Again, $\delta\Omega(h) = 0$ if and only if the functional Ω is appropriate to solve the non steady state problem, and this can be shown here. We also have the functionals :

$$\Omega(v_i) = \int_R \left[K_{ik}^{-1} \left(\frac{1}{2} v_k - v_0 \right) * v_i + \frac{1}{2S_s} * \frac{\partial v_i}{\partial x_i} * \frac{\partial v_k}{\partial x_k} \right] dR - \int_{A_1} (h_0 - H) * v_i * n_i \, dA - \int_{A_2} \frac{1}{S_s} * (v_i n_i - V) * \frac{\partial v_k}{\partial x_k} \, dA$$

$$\Omega(h, v_i) = \int_R \left[1 * v_i * \frac{\partial h}{\partial x_i} + \frac{1}{2} * v_i * K_{ik}^{-1} v_k - S_s h * \left(\frac{1}{2} h - h_0 \right) \right] dR - \int_{A_1} 1 * (h - H) * v_i * n_i \, dA + \int_{A_2} 1 * V * h \, dA$$

METHODS OF MINIMISATION OF FUNCTIONAL Ω

There are several methods : RITZ, COURANT, KANTOROVITCH, steepest descent...
RITZ's Method is the most common and will be presented.

RITZ'S METHOD

Definition of an operator

The governing equation of flow in R , can be written more simply :

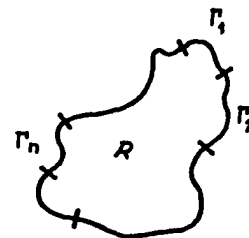
$$Ah(x_i, t) = f(x_i, t)$$

A is an operator $\left[\text{e.g. : } \frac{\partial}{\partial x} \quad : \quad \frac{\partial h}{\partial x} = Ah \right]$ and f is a given function (e.g. recharge).

The boundary conditions can also be written :

$$G_n h(x_i, t) = g_n(x_i, t) \text{ on } \Gamma_n$$

G_n is also an operator, and g_n a given function.



Exemple : $K_{ij} \frac{\partial h}{\partial x_j} n_i = -V$

$$G_n \equiv K_{ij} \frac{\partial}{\partial x_j} n_i$$

$$g_n \equiv -V$$

Definition of the inner product

For 2 functions u, v defined on a region R , the inner product is defined by :

$$\langle u, v \rangle = \int_R uv dR$$

The inner product with convolution is

$$\langle u * v \rangle = \int_R u * v dR$$

Self adjoint operators (symmetric operators)

$$\langle Au, v \rangle = \langle u, Av \rangle \quad \text{when } A \text{ is differential}$$

$$\langle Au * v \rangle = \langle u * Av \rangle \quad \text{when } A \text{ involves convolution,}$$

for any pair of sufficiently smooth function u and v satisfying the equivalent homogeneous boundary conditions of a given problem.

Basic assumptions of RITZ' Method

with the equations

$$\left\{ \begin{array}{ll} Ah = f & \text{on } R \\ G_n h = g_n & \text{on } \Gamma \end{array} \right.$$

the equivalent variational principle is to find the minimum of the functional $\Omega(h)$. Using RITZ' method, we will make the following assumptions.

- a) Operator A is self adjoint and positive bounded below
- b) Operator A is linear : this is not strictly necessary with RITZ' method, but will be assumed here
- c) One can use as an approximation of the true function h a finite serie h^N of the form :

$$h^N(x_1, t) = \sum_{n=1}^N a_n(t) \xi_n(x_1) \quad (\text{summation : } n = 1, 2 \dots N)$$

$a_n(t)$ are called the RITZ coefficients. They are constant in steady state.

$\xi_n(x_1)$ are called coordinate functions, or generalised coordinates. They are linearly independent. They form a basis for an N-dimensional subspace of a Hilbert space.

As h belongs to a Hilbert space, an infinite series would be necessary in order to have an exact expression of h in this way. The quality of the approximation is governed by the magnitude of N.

For any given N, the best approximation of the true function h by the function h^N can be shown to be the one that minimizes the functional Ω :

For example, if we can have a sufficient approximation of the true solution with $N = 1$ ($h^1 = a_1 \xi_1$), it will be obtained by minimizing $\Omega(h^1)$. This can be done by writing :

$$\frac{\partial \Omega(a_1 \xi_1)}{\partial a_1} = 0 \quad ; \quad a_1 = \text{constant.}$$

With $N = 2$, we obtain the best estimate $h^2 = a_1 \xi_1 + a_2 \xi_2$ of the true function h by minimizing $\Omega(h^2)$, that is to say

$$\left\{ \begin{array}{l} \frac{\partial \Omega(a_1 \xi_1 + a_2 \xi_2)}{\partial a_1} = 0 \quad ; \quad a_1 = \text{constant} \\ \frac{\partial \Omega(a_1 \xi_1 + a_2 \xi_2)}{\partial a_2} = 0 \quad ; \quad a_2 = \text{constant} \end{array} \right.$$

and so on for h^N .

FOUR MAJOR PROBLEMS

- a) What is the best way for choosing $\xi(x_i)$ in the region R ?
- b) As in an aquifer there exist 2 kinds of boundary conditions, how to have the $\xi_n(x_i)$ satisfy these boundary conditions for every shape of those boundary ?
 ex. : $\xi_1 = \sin(x)$, $\xi_2 = \sin^2(x)$ will not fit a given boundary condition ($h = H$ for instance) on any shape of the limit.
- c) How to write with mathematical expressions the functions f on R, and g_n , H , V on Γ , and how to treat these expressions ?
- d) If the transmissivity varies in R, how to choose the ξ_i to fullfill this obligation ?

FINITE ELEMENT RESPONSE TO THESE PROBLEMS

We take a finite number of finite elements and try to solve the problem independently in each of these elements, and then to combine together the different solutions.

A grid is thus introduced in RITZ' method. But in finite element, we will calculate an integral over the surface of the element, while in finite differences we have a partial differential equation that is applied at a point of each element

CONVERGENCE

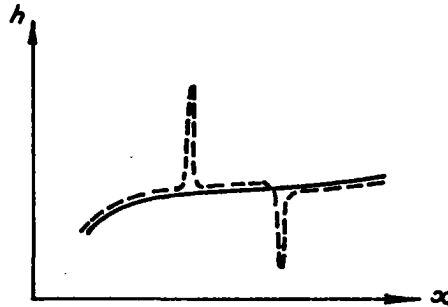
Problems come with the convergence of h^N towards h when N increases.

- Uniform convergence is $|h^N - h| \xrightarrow[N \rightarrow \infty]{} 0 \quad \forall x_i \in R$

- convergence in the mean is $\int_R (h^N - h)^2 dR \xrightarrow[N \rightarrow \infty]{} 0$

In uniform convergence, $h^N \rightarrow h$ for any x_1 .

With convergence in the mean, it is possible that h^N be very different of h in some points :



Uniform convergence always implies convergence in the mean, but not vice-versa ; convergence in the mean is faster than uniform convergence, because uniform convergence must be exact at each point of R . Faster means here that the number N of terms need not be so high.

Finite elements methods insure only convergence in the mean. Therefore, we are not sure to get good solution everywhere.

(cf. MIKHLIN, a russian scientist, 3 books translated into English. Base of variational principle).

DETERMINATION OF THE ξ_n

Problem : find h^N represented by a sequence $a_n \xi_n$

$$h^N = a_n \xi_n$$

We associate with each node n , whose global coordinates are X_i^n , a region R^n including all the neighboring elements, and a global coordinate function $\xi_n(X_i)$ defined by :

$$\xi_n(X_i^m) = \delta_{nm} \quad (\text{Kronecker } \delta)$$

$$\xi_n(X_i) = 0 \quad \forall X_i \in R^n$$

$$\xi_n \text{ varies linearly inside } R^n$$

ξ_n is called the pyramidal or "chapeau" function

Consequences :

1) $h^N = h_n \xi_n$ (Lagrange interpolation scheme)

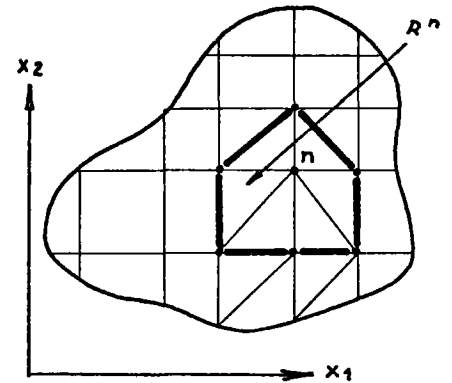
The "RITZ coefficients" are equal to the value of h^N at each node.

2) One deals only with linear functions

3) It is easy to satisfy boundary conditions where h is prescribed : some "Ritz coefficients" are thus determined "a priori".

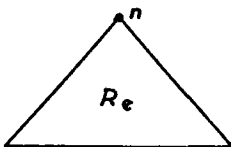
4) The matrix contains a great number of zeros which makes the resolution easier.

5) One can treat each element separately and assemble them later. This will be shown below.



LOCAL BEHAVIOUR

In each element, R^e , one defines local coordinate functions ξ_n^e linear on the element and satisfying:



$$\xi_n^e(x_i^m) = \delta_{nm}$$

$$\xi_n^e(x_i) = 0 \quad \forall x_i \notin R^e$$

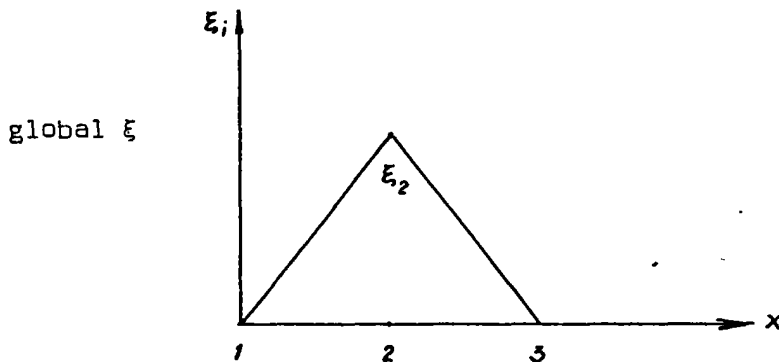
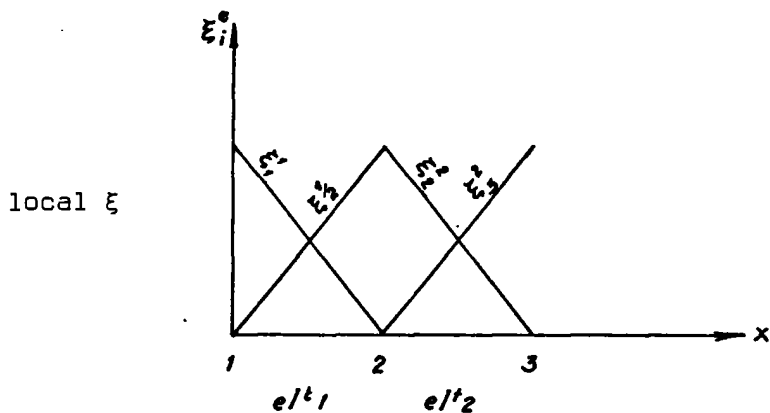
Each local coordinate function is a face of the pyramid which represents the global coordinate function. This can be written :

$$\xi_n(x_i) = \bigcup_e \xi_n^e(x_i)$$

\cup = unions, which means

$$\begin{cases} \xi_n(x_i) = \xi_n^e(x_i), & x_i \in R^e \\ \xi_n(x_i) = 0, & \forall x_i \notin R^e \end{cases}$$

Example : one-dimensional problem



$$\xi_2 = \xi_2^1 \cup \xi_2^2$$

One can write

$$h^N = h_n \xi_n \quad \text{global coordinates}$$

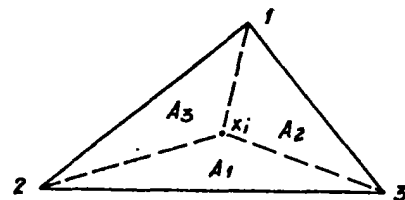
$$\text{or } h^N = h_n \bigcup_e \xi_n^e \quad \text{local coordinates}$$

LOCAL COORDINATES IN A TRIANGLE

They can be expressed by the natural coordinates

$$\phi_n(x_i) = \frac{A_n(x_i)}{A}$$

ϕ_n is a linear function having the same properties as ξ_n^e



$$A = A_1 + A_2 + A_3 = \text{triangle area}$$

If X_i is on point 1 $A_1 = A$ $A_2 = A_3 = 0 \implies \phi_1 = 1$ $\phi_2 = \phi_3 = 0$

RELATIONS BETWEEN ξ_n^e AND X_i (see annexe paper p. 8)

$$\begin{bmatrix} 1 \\ X \\ Y \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 \\ X^1 & X^2 & X^3 \\ Y^1 & Y^2 & Y^3 \end{bmatrix} \begin{bmatrix} \xi_1^e \\ \xi_2^e \\ \xi_3^e \end{bmatrix}$$

VALUES OF INTEGRALS OF ξ_1^e OVER A TRIANGLE

An interesting property of the local coordinate functions is that their integrals over a triangle depend only on the area of the triangle and not on its shape.

Example :

$$I = \int_{\Delta} \xi_1^e \, dR$$

Changing the variables to compute $dR = dx dy$ we get

$$dx \, dy = \begin{vmatrix} \frac{\partial x}{\partial \xi_1} & \frac{\partial x}{\partial \xi_2} \\ \frac{\partial y}{\partial \xi_1} & \frac{\partial y}{\partial \xi_2} \end{vmatrix} d\xi_1 \, d\xi_2 = 2A \, d\xi_1 \, d\xi_2$$

$$I = 2A \iint_{\Delta} \xi_1 \, d\xi_1 \, d\xi_2 = 2A \int_0^1 d\xi_2 \int_0^{1-\xi_2} \xi_1 \, d\xi_1 = - \left[2A \left(\frac{1-\xi_2}{6} \right)^3 \right]_0^1 = \frac{A}{3}$$

For other integrals of this kind see tables of FELIPPA.

MINIMIZATION OF THE FUNCTIONAL

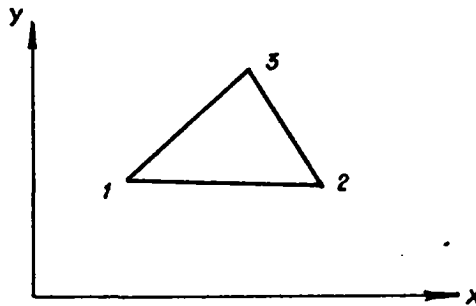
$$\Omega(h) = \int_R \frac{1}{2} K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial h}{\partial x_i} \, dR - \int_{A_1} (h-H) K_{ij} \frac{\partial h}{\partial x_j} n_i \, dA + \int_{A_2} Vh \, dA$$

This may be considered as the total energy in R which we will minimize. In fact the functional that we shall minimize will not contain the integral over A_1 : in the finite element method it is possible to impose very simply this boundary condition by prescribing $h = H$ on the nodes of A_1 .

$$\Omega(h) = \int_R \frac{1}{2} K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial h}{\partial x_i} dR + \int_{A_2} V h dA$$

Elements

R is divided generally into quadrilaterals or triangles ; but each quadrilateral is divided into four triangles, so that the basic element is always a triangle



Assumption : the head h is a linear function of the coordinates in the triangle:

$$h = a + bX + cY$$

a, b, c are calculated by writing this equation at the three nodes of the triangle

$$h_1 = a + bX_1 + cY_1$$

$$h_2 = a + bX_2 + cY_2$$

$$h_3 = a + bX_3 + cY_3$$

This gives the formula

$$h = \frac{1}{2A} \left[(a_1 + b_1X + c_1Y)h_1 + (a_2 + b_2X + c_2Y)h_2 + (a_3 + b_3X + c_3Y)h_3 \right]$$

$$\begin{aligned}
 \text{with : } \quad a_1 &= X_2 Y_3 - X_3 Y_2 & b_1 &= Y_2 - Y_3 & c_1 &= X_3 - X_2 \\
 a_2 &= X_3 Y_1 - X_1 Y_3 & b_2 &= Y_3 - Y_1 & c_2 &= X_1 - X_3 \\
 a_3 &= X_1 Y_2 - X_2 Y_1 & b_3 &= Y_1 - Y_2 & c_3 &= X_2 - X_1
 \end{aligned}$$

$$2A = c_2 b_1 - c_1 b_2$$

We define the local coordinate functions ξ_n^e :

$$\xi_n^e = \frac{1}{2A} (a_n + b_n X + c_n Y)$$

h is thus approximated by $h^N = h_n \cup_e \xi_n^e$; it can be verified that the ξ_n are coordinate functions as those defined earlier.

For this h^N the functional can be written

$$\Omega(h^N) = \Omega(h_n \cup_e \xi_n^e) = \sum_e \Omega(h_n \xi_n^e) = \sum_e \Omega^e(h)$$

because the integrals over the whole region R can be taken separately over each element :

$$\Omega^e(h) = \frac{1}{2} \int_{R^e} K_{ij} \frac{\partial \xi_m^e}{\partial x_j} h_m \frac{\partial \xi_n^e}{\partial x_i} h_n \, dR^e + \int_{A_2^e} V \xi_n^e h_n \, dA^e$$

and minimizing this expression we get :

$$\frac{\partial \Omega^e(h)}{\partial h_n} = K_{ij} \int_{R^e} \frac{\partial \xi_n^e}{\partial x_j} \frac{\partial \xi_m^e}{\partial x_i} h_m \, dR^e + \int_{A_2^e} V \xi_n^e \, dA^e = 0$$

Let us define the matrix :

$$A_{nm}^e = K_{ij} \int_{R^e} \frac{\partial \xi_n^e}{\partial x_j} \frac{\partial \xi_m^e}{\partial x_i} \, dR^e$$

Then for the entire system it comes :

$$\frac{\partial \Omega(h)}{\partial h_n} = \sum_e \left[AA_{nm}^e h_m + \int_{A_2^e} V \xi_n^e dA^e \right] = 0$$

CALCULATION OF THE MATRIX A_{nm}^e

$$A_{nm}^e = \int_{R^e} K_{ij} \frac{\partial \xi_n^e}{\partial x_j} \frac{\partial \xi_m^e}{\partial x_i} dR^e$$

$$A_{nm}^e = \int_{\Delta} \left[K_{xx} \frac{\partial \xi_n^e}{\partial x} \frac{\partial \xi_m^e}{\partial x} + K_{xy} \frac{\partial \xi_n^e}{\partial x} \frac{\partial \xi_m^e}{\partial y} + K_{yx} \frac{\partial \xi_m^e}{\partial x} \frac{\partial \xi_n^e}{\partial y} + K_{yy} \frac{\partial \xi_n^e}{\partial y} \frac{\partial \xi_m^e}{\partial y} \right] dx dy$$

$$\xi_n^e = \frac{1}{2A} (a_n + b_n x + c_n y)$$

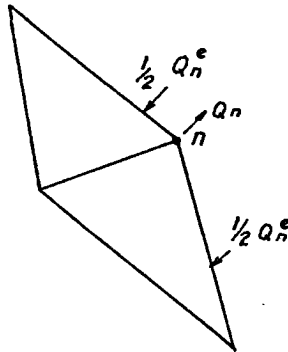
$$A_{nm}^e = \frac{1}{4A^2} \int_{\Delta} (K_{xx} b_n b_m + K_{xy} c_n b_m + K_{yx} b_n c_m + K_{yy} c_n c_m) dx dy$$

$$A_{nm}^e = \frac{1}{4A} (K_{xx} b_n b_m + K_{xy} c_n b_m + K_{yx} b_n c_m + K_{yy} c_n c_m)$$

With axisymmetric problems AA_{nm}^e is multiplied by $2\pi \left[\frac{r_1 + r_2 + r_3}{3} \right]$

CALCULATION OF $\int_{A_2^e}$

$$\int_{A_2^e} V \xi_n^e dA^e = V \int_{A_2^e} \xi_n^e dA^e = V \left[\frac{1+0}{2} \right] A^e = -\frac{1}{2} Q_n^e$$



Let us define the global matrix for the entire system

$$A_{nm} = \sum_e A_{nm}^e$$

$$Q_n = \sum_e \frac{1}{2} Q_n^e$$

$$A_{nm} h_m = Q_n$$

The solution of this set of linear equations gives the value of the head h_m at each node of the grid.

OTHER FUNCTIONALS Ω

We can resume the different expressions of Ω when this term is expressed in function of h (head) or/and v_i (velocity) in steady state and non-steady state.

1) Steady state - Ω in terms of h

$$\Omega(h) = \int_R \frac{1}{2} K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial h}{\partial x_i} dR - \int_{A_1} (h-H) K_{ij} \frac{\partial h}{\partial x_j} n_i dA + \int_{A_2} V \cdot h \cdot dA$$

2) Steady state - Ω in terms of h and v_i

$$\Omega(h, v_i) = \int_R \left[v_i \frac{\partial h}{\partial x_i} + \frac{1}{2} v_i K_{ik}^{-1} v_k \right] dR - \int_{A_1} (h-H) v_i n_i dA + \int_{A_2} V \cdot h \cdot dA$$

3) Non-steady state - Ω in terms of h

$$\begin{aligned} \Omega(h) = & \int_R \left[\frac{1}{2} * K_{ij} \frac{\partial h}{\partial x_j} * \frac{\partial h}{\partial x_i} + S_s h * \left(\frac{1}{2} h - h_o \right) \right] dR \\ & - \int_{A_1} 1 * (h-H) * K_{ij} \frac{\partial h}{\partial x_j} n_i dA + \int_{A_2} 1 * V * h \cdot dA \end{aligned}$$

4) Non steady state - Ω in terms of v_i

$$\begin{aligned} \Omega(v_i) = & \int_R \left[K_{ik}^{-1} \left(\frac{1}{2} v_k - v_{ko} \right) * v_i + \frac{1}{2S_s} * \frac{\partial v_i}{\partial x_i} * \frac{\partial v_k}{\partial x_k} \right] dR \\ & - \int_{A_1} (h_o - H) * v_i * n_i dA - \int_{A_2} \frac{1}{S_s} * (v_i n_i - V) * \frac{\partial v_k}{\partial x_k} dA \end{aligned}$$

5) Non steady state - Ω in terms of h and v_i

$$\begin{aligned} \Omega(h, v_i) = & \int_R \left[1 * v_i * \frac{\partial h}{\partial x_i} + \frac{1}{2} * v_i * K_{ik}^{-1} v_s - S_s h * \frac{1}{2} (h-h_o) \right] dR \\ & - \int_{A_1} 1 * (h - H) * v_i * n_i dA + \int_{A_2} 1 * V * h dA \end{aligned}$$

For unsteady state, Ω may be written :

$$\Omega(h) = \int_R \left[\frac{1}{2} * K_{ij} \frac{\partial h}{\partial x_i} * \frac{\partial h}{\partial x_i} + S_s \left(\frac{h}{2} * h - h * h_0 \right) \right] dR \quad (1)$$

$$- \int_{A_1} 1 * (h - H) * K_{ij} \frac{\partial h}{\partial x_j} n_i dA + \int_{A_2} (1 * V * h) dA \quad (2) \quad (3)$$

For steady state, we don't take care of term (2) expressed along A_1 , because the head is fixed and this term does not change.

For one element e, the functional becomes, using $h = N_n h_n$ $N_n = \xi_n^e$

$$\Omega^e(h) = \int_{R^e} \left[\frac{1}{2} * K_{ij} \frac{\partial N_n}{\partial x_j} h_n * \frac{\partial N_m}{\partial x_i} h_m + S_s \left(\frac{1}{2} N_n h_n * N_m h_m - N_n h_n * N_n h_{om} \right) \right] dR$$

$$+ \int_{A_2^e} (1 * V * N_n h_n) dA$$

So the first variation is :

$$\delta \Omega(\tilde{h}) = \int_{R^e} \left[1 * K_{ij} * \frac{\partial N_m}{\partial x_j} \frac{\partial N_n}{\partial x_i} h_m + 1 * S_s N_n N_m (h_m - h_{om}) \right] dR^e + \int_{A_2^e} (1 * V * N_n) dA^e$$

We can put out the convolution inside the different terms.

$$\delta \Omega(\tilde{h}) = \left[\int_{R^e} 1 * K_{ij} \frac{\partial N_n}{\partial x_j} \frac{\partial N_m}{\partial x_i} h_m + S_s N_n N_m (h_m - h_{om}) dR^e + \int_{A_2^e} (1 * V N_n) dA^e \right] * 1 =$$

The term on left hand side of the convolution must be equal to zero, so :

$$0 = \int_{R^e} \left[K_{ij} \frac{\partial N_n}{\partial x_j} \frac{\partial N_m}{\partial x_i} * h_m + S_s N_n N_m (h_m - h_{om}) \right] dR^e + \int_{A_2^e} (1 * V N_n) dA^e$$

The expression of the matrix AA_{nm}^e is

$$AA_{nm}^e \equiv K_{ij} \int_{R^e} \frac{\partial N_n}{\partial x_j} \frac{\partial N_m}{\partial x_i} dR^e$$

We introduce a new term D_{nm}^e

$$D_{nm}^e \equiv S_s \int_{R^e} N_n N_m dR^e \quad \text{For the value of these terms, we may use the table of local integrals over triangles}$$

With the table of values, we can get immediately the value of D_{nm}^e . This value is defined by the geometry

$$D_{nm}^e = \begin{cases} S_s A \frac{1}{12} & (n \neq m) \\ S_s A \frac{2}{12} & (n = m) \end{cases}$$

We can evaluate

$$\int_{A_2^e} V N_n dA^e = \frac{1}{2} Q_n^e$$

For the entire region, we obtain all the terms for integral calculus.

$$\left\{ \begin{array}{l} AA_{nm} \equiv \sum_e AA_{nm}^e \\ Q_n \equiv \sum_e Q_n^e \\ D_{nm} \equiv \sum_e D_{nm}^e \end{array} \right.$$

The integral becomes now

$$D_{nm} (h_n - h_{om}) + AA_{nm} * h_m - 1 * Q_n = 0$$

$$1 * h_m = \int_{t-\Delta t}^t h_m(\tau) d\tau \quad \text{with the assumptions that } h \text{ varies linearly with } x_i \text{ and with time :}$$

$$1 * h_m \approx \frac{\Delta t}{2} [h_m(t) + h_m(t-\Delta t)]$$

Δt must be ^{an} appropriately small time increment.

Another assumption is that Q has linear variations with time

$$1 * Q_n = \frac{\Delta t}{2} (Q_n(t) + Q_n(t-\Delta t)) = \Delta t \bar{Q}_n$$

Hence these two expressions permit to eliminate the convolutions in the integral

$h_m(t-\Delta t) = h_{om}$ is the original head used in this time step.

After the different simplifications, the expression becomes :

$$D_{nm} \left[h_m(t) - h_m(t-\Delta t) \right] + AA_{nm} \cdot \frac{\Delta t}{2} \left[h_m(t) + h_m(t-\Delta t) \right] = \Delta t \overline{Q}_n$$

$$D_{nm} \left[h_m(t) + h_m(t-\Delta t) - 2h_m(t-\Delta t) \right] + AA_{nm} \cdot \frac{\Delta t}{2} \left[h_m(t) + h_m(t-\Delta t) \right] = \Delta t \overline{Q}_n$$

$$\frac{1}{2} \left[h_m(t) + h_m(t-\Delta t) \right] \left[D_{nm} + AA_{nm} \cdot \frac{\Delta t}{2} \right] = \frac{\Delta t}{2} \cdot \overline{Q}_n + \frac{2}{2} D_{nm} \cdot h_m(t-\Delta t)$$

A_{nm} will be defined as the term :

$$A_{nm} \equiv D_{nm} + AA_{nm} \frac{\Delta t}{2} \quad \text{for unsteady state (for steady state } AA_{nm} \text{ only)}$$

using $B_n \equiv D_{nm} h_m(t - \Delta t) + \frac{\Delta t}{2} \overline{Q}_n$

and $X_m \equiv \frac{1}{2} \left[h_m(t) + h_m(t - \Delta t) \right]$

for steady state we had

$$AA_{nm} h_m = Q_n$$

for non steady state

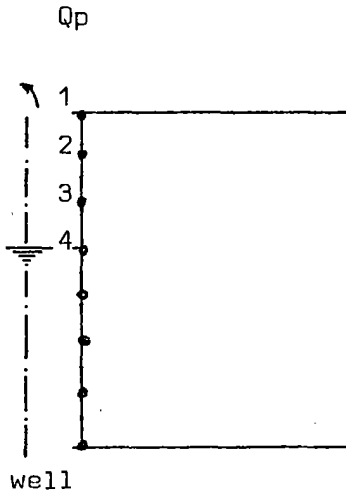
$$AA_{nm} X_m = B_n$$

It will be proved later that D_{nm} can be changed into a vector for better results.

DISCUSSION OF THE EQUATION FOR NON-STEADY STATE AND EVALUATION OF BOUNDARY CONDITIONS

We reduce the number of equations from N to N-K where K is the number of nodes where the head is known.

For example, one advantage of this method appears in considering a partially-penetrating well with some constant pumping rate Qp.



In the well-bore $h = f(t)$

At any instant of time, we have

$$h_1 = h_2 = h_3 = h_4 = ?$$

The term X_n includes $h_m(t)$ et $h_m(t-\Delta t)$ which are constant at any instant of time

so

$$A_{11}h_1 + A_{12}h_2 + A_{13}h_3 + A_{14}h_4 + \dots = B_1$$

$$A_{21}h_1 + \dots + A_{24}h_4 + \dots = B_2$$

$$A_{31}h_1 + \dots + A_{34}h_4 + \dots = B_3$$

$$A_{41}h_1 + \dots + A_{44}h_4 + \dots = B_4$$

$$A_{51}h_1 + \dots + \dots + \dots = \dots$$

A_{ij} depends on geometry and different h_i are equal in the equations : the 4 first equations may be reduced to one equation

$$(A_{11} + A_{12} + A_{13} + A_{14})h_1 + A_{15}h_5 + \dots = B_1$$

$$(A_{51} + A_{52} + A_{53} + A_{54})h_1 + A_{55}h_5 + \dots = B_5$$

$$(A_{61} + \dots + A_{64})h_1 + \dots = B_6$$

But $Q_p = Q_1 + Q_2 + Q_3 + Q_4$ at any instant of time

We guess Q_1 - then we must calculate Q_2, Q_3 and Q_4

The result $Q_{cal} = Q_1 + Q_2 + Q_3 + Q_4$ is generally not equal to Q_p

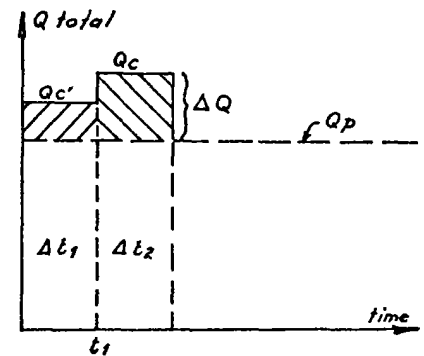
Hence the value of head can be defined by

$$h_m(t) = \frac{Q_p}{Q_{calculated}} \times h_{m,calculated}(t)$$

only for the first time step

EXTENSION FOR SEVERAL TIME STEPS

At the end of the first time step Q_{cal} is generally not equal to Q_p : so, we adjust h_m . At the end of the second time step, equal to the first time step $\Delta t_2 = \Delta t_1$, the flow may be also different of Q_p .



At point m (node), we have : (cal \equiv calculated)

$$(h_2)_{cal} = \frac{Q_p}{4\pi T} \left(W(t_2 - 0) \right) + \frac{\overbrace{Q_c - Q_p}^{\Delta Q}}{4\pi T} \left(W(t_2 - t_1) \right)$$

$$\text{with } W(t_2 - 0) = \int_u^\infty \frac{e^{-y}}{y} dy - \int_0^\infty \frac{e^{-y}}{y} dy \quad \text{with } u = \frac{s_s r^2}{4Kt_2}$$

As $\Delta t_2 = \Delta t_1$, the value of $t_2 - t_1$ is : $t_2 - t_1 = t_1 - 0$

The value of $(h_2)_{cal}$ is, in this case :

$$(h_2)_{cal} = \frac{Q_p}{4\pi T} \left(W(t_2 - t_1) + W(t_1 - 0) \right) + \frac{Q_c - Q_p}{4\pi T} W(t_1 - 0) \frac{Q_p}{Q_p}$$

where $Q_p \cdot \frac{W(t_1 - 0)}{4\pi T}$ has been calculated at first time step

$$\begin{aligned} (h_2)_{cal} &= (h_2 - h_1)_{correct} + (h_1)_{correct} + \frac{Q_c - Q_p}{Q_p} \cdot (h_1)_{correct} \\ &= (h_2)_{correct} + \frac{Q_c - Q_p}{Q_p} \cdot (h_1)_{correct} \end{aligned}$$

The value of h_1 in the right hand side has been obtained after the first time step.

Finally :

$$(h_2)_{correct} = (h_2)_{cal} - \frac{Q_c - Q_p}{Q_p} \cdot (h_1)_{correct}$$

For the third time step, we use

$$\Delta t_3 = \Delta t_2 + \Delta t_1 \quad \dots \text{ and so on } \dots$$

STEADY STATE - FREE SURFACE

We introduce 2 new boundaries

- seepage face
- free surface face

so we have 4 kinds of boundaries.

$$\frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j} \right) = 0 \quad (1)$$

$$h = H \text{ on } A_1 \quad (2)$$

$$K_{ij} \frac{\partial h}{\partial x_j} n_i = -V \text{ on } A_2 \quad (3)$$

Such are conditions for confined flow.

For the seepage face, if we know the geometry of this face,

$$h = x_3 \text{ on } S \quad (4)$$

If there is no infiltration, the free surface has a steady position.

$$h = \eta \text{ on F.S.} \quad (5)$$

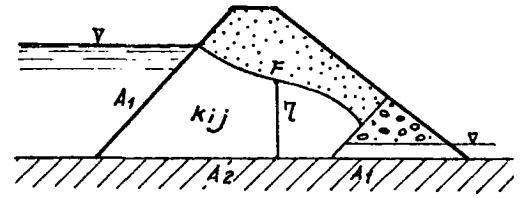
$$K_{ij} \frac{\partial h}{\partial x_j} n_i = I n_3 \text{ on F.S.} \quad (6) \text{ Infiltration is positive downward.}$$

The determination of the intersection of the free surface with the seepage face is the main problem.

Determination of a functional

$$\begin{aligned} \Omega(h, \eta) = & \int_R \frac{1}{2} K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial h}{\partial x_i} dR \quad (T1) - \int_{A_1} (h-H) K_{ij} \frac{\partial h}{\partial x_j} n_i dA \quad (T2) \\ & - \int_S (h-x_3) K_{ij} \frac{\partial h}{\partial x_j} n_i dA \quad (T3) + \int_{A_2} V \cdot h \cdot dA \quad (T4) - \int_F (h-\eta) K_{ij} \frac{\partial h}{\partial x_j} n_i dA \quad (T5) \\ & - \int_F \eta I n_3 dA \quad (T6) \end{aligned}$$

Hence, terms of this functional are similar to those of the functional for steady state in a confined aquifer.



Let us introduce a perturbation in the value of h and η and

take the derivative of Ω at point (h, η)

$$\begin{aligned} \frac{d}{d\lambda} \Omega(h+\lambda\tilde{h}, \eta+\lambda\tilde{\eta}) \Big|_{\lambda=0} &= \delta\Omega(h+\lambda\tilde{h}, \eta+\lambda\tilde{\eta}) \Big|_{\lambda=0} \\ \Omega(h+\lambda\tilde{h}, \eta+\lambda\tilde{\eta}) &= \int_R \frac{1}{2} K_{ij} \frac{\partial(h+\lambda\tilde{h})}{\partial x_j} \frac{\partial(h+\lambda\tilde{h})}{\partial x_i} dR - \int_{A_1} (h+\lambda\tilde{h}-H) K_{ij} \frac{\partial(h+\lambda\tilde{h})}{\partial x_j} n_i dA \\ &- \int_S (h+\lambda\tilde{h}-X_3) K_{ij} \frac{\partial(h+\lambda\tilde{h})}{\partial x_j} n_i dA + \int_{A_2} V(h+\lambda\tilde{h}) dA - \int_F (h+\lambda\tilde{h}-\eta-\lambda\tilde{\eta}) K_{ij} \frac{\partial(h+\lambda\tilde{h})}{\partial x_j} n_i dA \\ &- \int_F (\eta+\lambda\tilde{\eta}) I n_3 dA \end{aligned}$$

The first variation $\delta\Omega(h+\lambda\tilde{h}, \eta+\lambda\tilde{\eta})$ at $\lambda = 0$ is :

$$\begin{aligned} \frac{d\Omega}{d\lambda} \Big|_{\lambda=0} &= \int_R K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial \tilde{h}}{\partial x_i} dR - \int_{A_1} \left[(h-H) K_{ij} \frac{\partial \tilde{h}}{\partial x_j} + \tilde{h} K_{ij} \frac{\partial h}{\partial x_j} \right] n_i dA \\ &- \int_S \left[(h-X_3) K_{ij} \frac{\partial \tilde{h}}{\partial x_j} + \tilde{h} K_{ij} \frac{\partial h}{\partial x_j} \right] n_i dA + \int_{A_2} V \tilde{h} dA \\ &- \int_F \left[(h-\eta) K_{ij} \frac{\partial \tilde{h}}{\partial x_j} + (\tilde{h}-\tilde{\eta}) K_{ij} \frac{\partial h}{\partial x_j} \right] n_i dA - \int_F \tilde{\eta} I n_3 dA \end{aligned}$$

Using GREEN's first identity, with the two terms $K_{ij} \frac{\partial h}{\partial x_j}$ and \tilde{h} , we replace the first integral by

$$\begin{aligned} \int_R K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial \tilde{h}}{\partial x_i} dR &= - \int_R \tilde{h} \frac{\partial}{\partial x_i} K_{ij} \frac{\partial h}{\partial x_j} dR + \int_{A_1} \tilde{h} K_{ij} \frac{\partial h}{\partial x_j} n_i dA \\ &+ \int_S \tilde{h} K_{ij} \frac{\partial h}{\partial x_j} n_i dA + \int_{A_2} \tilde{h} K_{ij} \frac{\partial h}{\partial x_j} n_i dA + \int_F \tilde{h} K_{ij} \frac{\partial h}{\partial x_j} n_i dA \end{aligned}$$

We substitute this value of the integral in $\frac{d\Omega}{d\lambda} \Big|_{\lambda=0}$

Some terms disappear, the result being

after simplification

$$\begin{aligned} \delta\Omega(h, \eta) &= - \int_R \tilde{h} \frac{\partial}{\partial x_i} K_{ij} \frac{\partial h}{\partial x_j} dR - \int_{A_1} (h-H) K_{ij} \frac{\partial \tilde{h}}{\partial x_j} n_i dA \\ &- \int_S (h-X_3) K_{ij} \frac{\partial \tilde{h}}{\partial x_j} n_i dA + \int_{A_2} (K_{ij} \frac{\partial h}{\partial x_j} n_i + V) \tilde{h} dA \\ &- \int_F (h-\eta) K_{ij} \frac{\partial \tilde{h}}{\partial x_j} n_i dA + \int_F (K_{ij} \frac{\partial h}{\partial x_j} n_i - I n_3) \tilde{\eta} dA \end{aligned}$$

(E1) (E2) (E3) (E4) (E5) (E6)

This represents the first variation of Ω : the two conditions IF and ONLY IF are :

→ IF conditions (1) to (6) are satisfied $\Delta\Omega(h,\eta) = 0$

condition (1) satisfies member E_1 of the equation

"	(2)	"	"	E_2	")	
"	(3)	"	"	E_4	")	
"	(4)	"	"	E_3	")	so $\delta\Omega(h,\eta) = 0$.
"	(5)	"	"	E_5	")	
"	(6)	"	"	E_6	")	

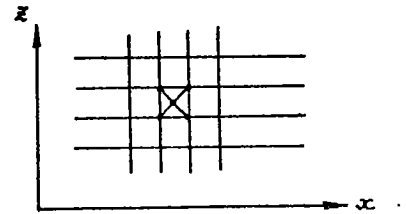
→ and ONLY IF these conditions are satisfied $\delta\Omega(h,\eta) = 0$ for every value of \tilde{h} , so all conditions (1) to (6) are satisfied.

Minimization :

With the basic assumption

$$h = a + bx + cz$$

the problem is similar to the precedent ones.



We have 2 variables h and η :

we cannot solve the problem directly ; so we proceed as follows :

step (1) - we take into account the prescribed head boundary conditions on F and S

step (2) - we take into account only the prescribed flux boundary conditions on F and S

⋮
and so on.

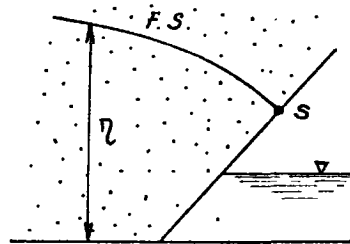
Example :

We fix the free surface; conditions (4) and (5) are satisfied)
 conditions (2) and (3) are easily satisfied) for
)
 we ignore condition (6))step(1)

(T2 drops for step (1) and (2) (cf. see expression of the functional
 { T3 " " (1) for the notations of the different
 { T5 " " (1) terms)
 { T6 is ignored for step (1)

We get a system $AA_{nm} h_m = Q_n$

In step (1), flux is calculated along the free surface and the seepage face : we get values of flux Q , along the free surface (Q_F) and the seepage face (Q_S). We set Q_F equal to the prescribed infiltration and maintain Q_S for step (2).



In second step, we have now flux along the free surface and the seepage face and can solve for head on F and S. F is then shifted to a new position if necessary (if $h \neq \eta$ on F).

The equation used in ~~the~~ first step is :

$$\Omega(h) = \int_R \frac{1}{2} K_{ij} \frac{\partial h}{\partial x_j} \cdot \frac{\partial h}{\partial x_i} dR + \int_{A_2} V \cdot h \cdot dA$$

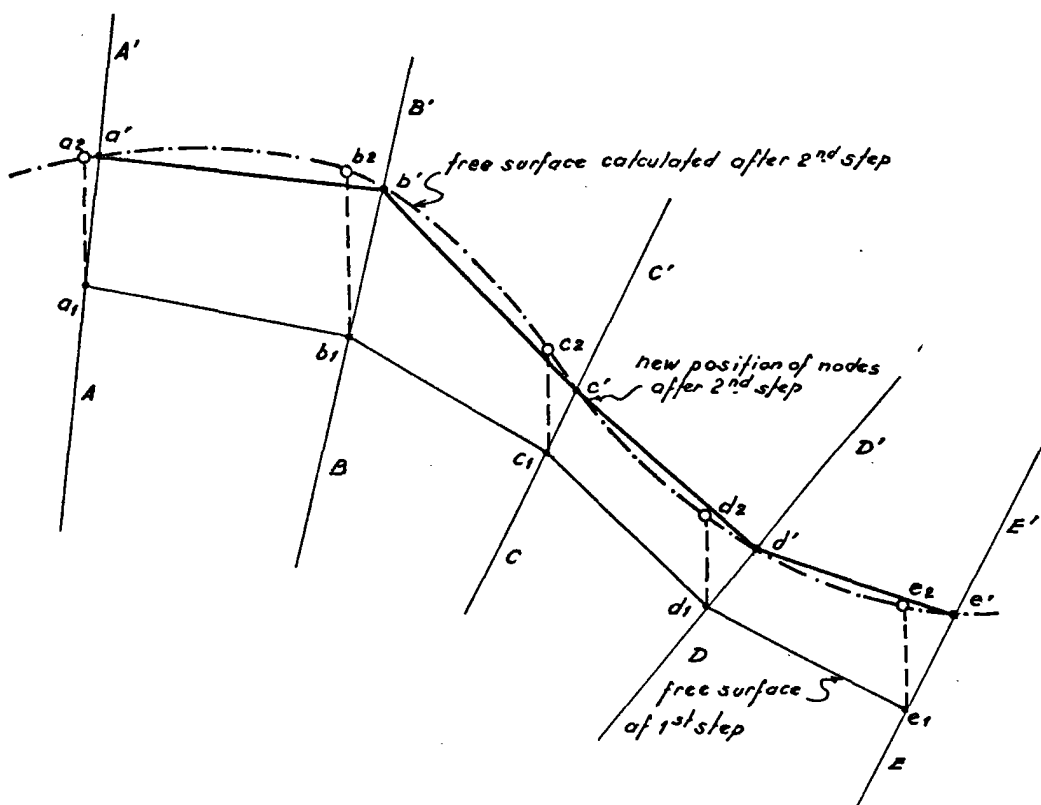
The equation used in ~~the~~ second step is :

$$\Omega(h) = \int_R \frac{1}{2} K_{ij} \frac{\partial h}{\partial x_j} \cdot \frac{\partial h}{\partial x_i} dR + \int_S h \cdot V_s \cdot dA + \int_{A_2} V \cdot h \cdot dA - \int_F h I n_3 dA$$

In these two steps, we keep the same shapes for the free surface and seepage faces.

Suppose that after step 2, we get a new calculation of values of head along the 2 faces

- on the free surface, the head must be equal to η (which is the vertical coordinate). We modify as shown below :



After step (2), we must move the free surface. But the change of positions of the different nodes must be done along the different directions AA' , BB' , ...

This condition is required by :

- the fact that different materials can be situated on either side of the directrice-line (as AA' , BB' , ...).
- the impossibility to move the free surface vertically if this surface becomes almost vertical.

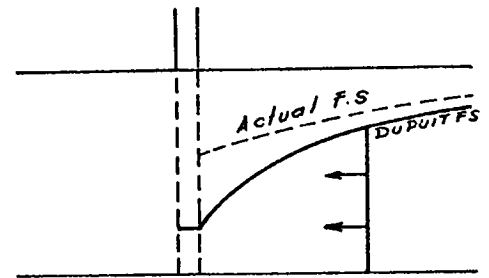
So the new position of nodes adopted after the second step is at the intersection of the theoretical new surface (dashed line) with the lines in directions AA' , BB' , ...

UNSTEADY FLOW WITH A FREE SURFACE : PROGRAM FREESURF II

First approach :

- Dupuit assumption
- Dupuit assumes that:

1) There is no seepage face, the free surface is recorded to the level of the water.



2) The direction of the Flow is everywhere horizontal.

3) The flow is proportional to the gradient of the free surface.

This gives rise to the Boussinesc equation :

$$\frac{\partial}{\partial x_i} \left(\underbrace{h K_{ij}}_{T_{ij}, \text{ variable with } h} \frac{\partial h}{\partial x_j} \right) = S_y \frac{\partial h}{\partial t}$$

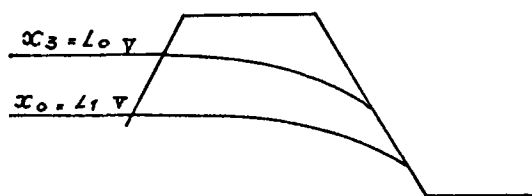
$S_y = \text{Specific yield} = \text{effective porosity}$

or :

$$\frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h^2}{\partial x_j} \right) = \frac{S_y}{h} \frac{\partial h^2}{\partial t}$$

This equation being non linear and difficult to solve, it is not always advantageous to use the Dupuit assumption.

Furthermore, it is not very good near a well, and simply would not work for the lowering of the water in a dam :



In this case, the flux across the free surface will not be zero or equal to the infiltration : it is a new kind of boundary condition.

Second approach :

We will use the equation

$$\frac{\partial}{\partial x_i} (K_{ij} \frac{\partial h}{\partial x_j}) = S_s \frac{\partial h}{\partial t}$$

S_s is the specific storage due to compressibility of the porous medium. It can be included in the computation, but is more or less negligible, and is not included in FREESURF II. Therefore we will write.:

$$(1) \frac{\partial}{\partial x_i} (K_{ij} \frac{\partial h}{\partial x_j}) = 0$$

This is a continuity equation for steady state.

$$(2) h(x_1, 0) = h_0(x_1)$$

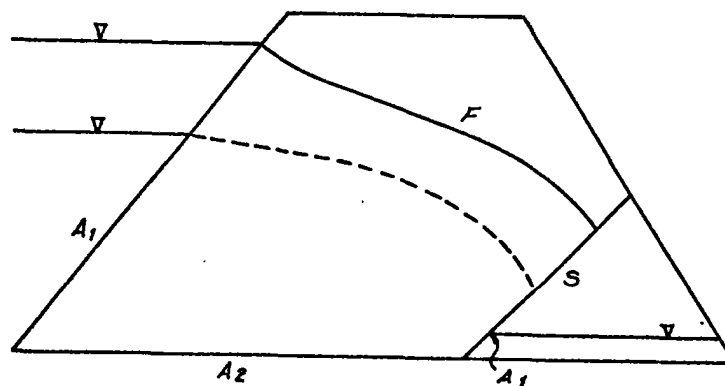
$$(3) \eta(x_1, x_2, 0) = \eta_0(x_1, x_2)$$

} initial conditions

η is the elevation of the free surface at the point of coordinates x_1, x_2 .

If $S_s = 0$ in equation (1), as in Freesurf II, it is not necessary to provide the initial condition (2) : the condition (3) provides the boundary of the flow region, where equation (1) would permit to determine in each point the flow and the head. But this calculation will even not be necessary.

Boundary conditions



$$A_1 : h(x_i, t) = H(x_i, t)$$

$$A_2 : K_{ij} \frac{\partial h}{\partial x_j} n_i = -V(x_k, t)$$

n_i is the unit outer normal vector across the boundary

$$F : \begin{cases} \eta(x_1, x_2, t) = h(x_1, x_2, \eta, t) \\ K_{ij} \frac{\partial h}{\partial x_j} n_i = (I - S_y \frac{\partial \eta}{\partial t} n_3) \end{cases}$$

n_3 is the vertical component of n_i

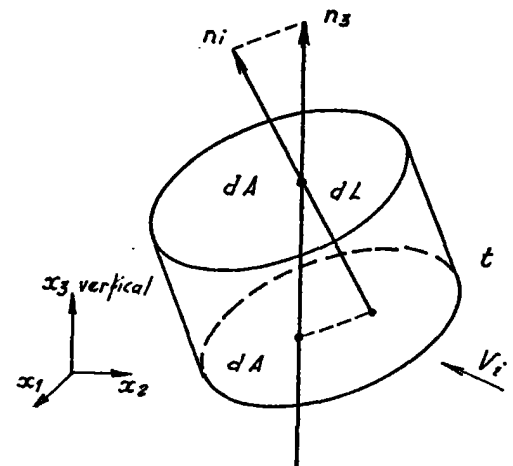
$$S : h(x_i, t) = X_3$$

Development of the equation of the free surface

Suppose that we have a rising free surface.

V_i is the usual velocity vector of Darcy.

The small element of surface dA rises between time t and $t + dt$; its displacement dL is measured along the direction of the unit vector n_i , assumed to be orthogonal to dA both at time t and $t + dt$.



The vertical component of dL is $\frac{\partial \eta}{\partial t} dt$. Let n_3 be the component of n_i in the vertical direction x_3 .

The amount of water stored in the three dimensional element of surface dA and thickness dL during the time increment dt is :

$$S_y dA dL = S_y dA \underbrace{\frac{\partial \eta}{\partial t} dt}_{dL} n_3$$

The amount of water entering into the element from below and from above is

$$(v_i n_i + I n_3) dA dt$$

The product $v_i n_i$ is the component of Darcy's specific flux perpendicular to the surface dA ; the other component parallel to dA does not participate to the movement of the free surface.

I is the rate of infiltration, which is a vertical flow.

Identifying those 2 terms, we obtain the second equation of the boundary condition on F .

It is this equation which introduces the non steady phenomenon into the steady state equation.

Third approach

Another way of solving the non steady flow is to use a succession of steady states.

- 1/ For a given position of the free surface, the corresponding steady state flow is computed.
- 2/ The Darcy velocity is computed at the free surface using this steady state. This velocity is not zero because the position of the free surface is not in a state of equilibrium.
- 3/ The free surface is moved for a given step Δt according to the in 2/ computed velocity :

$$\text{displacement} = \frac{V}{\phi} dt \quad \phi = \text{effective porosity.}$$

See - Herbert, 1968, in the journal "Groundwater". He used a RC network (electric analog).

- Szabo & Mc Craig, 1968, Bulletin of Water Research Association. They used a finite difference method.

- Parekh, 1967, with finite elements.
- Taylor, 1971, with finite elements, in the Journal of irrigation and drainage.

In this method, the previous free surface is used as the initial condition for each time step, i.e. the formulation is explicit, which brings stability problems : the free surface oscillates more and more as time increases, unless the time step is very small.

On the contrary, our 2nd approach is entirely implicit.

Variational principle for the second approach

$$\begin{aligned} \Omega(h, \eta) = & \int_R \frac{1}{2} K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial h}{\partial x_i} dR - \int_{A_1} (h - H) K_{ij} \frac{\partial h}{\partial x_j} n_i dA - \int_S (h - X_3) K_{ij} \frac{\partial h}{\partial x_j} n_i dA \\ & + \int_{A_2} V h dA - \int_F (h - \eta) K_{ij} \frac{\partial h}{\partial x_j} n_i dA - \int_F \eta (I - S_y \frac{\partial \eta}{\partial t}) n_3 dA \end{aligned}$$

As the finite element method directly satisfies the conditions $h = H$ on A_1 and $h = X_3$ on S , the integrals on A_1 and S disappear in the expression of the functional.

The main problem is that at a given time, we must have a fixed mesh in order to apply the finite element method : it is therefore not possible to insure directly the condition $h = \eta$ on F , and our variational principle is not applicable.

We cannot use convolution in our expressions, because it requires the region R to be constant.

The procedure that we will use ^{is} to assume initially that $\frac{\partial \eta}{\partial t}$ is known, and to iterate.

Let us calculate the first variation of Ω

$$\delta\Omega(h,\eta) = \frac{d}{d\lambda} \Omega(h + \lambda\tilde{h}, \eta + \lambda\tilde{\eta}) \Big|_{\lambda=0}$$

Substituting h and η by $h + \lambda\tilde{h}$, $\eta + \lambda\tilde{\eta}$, but not for the term $\frac{\partial\eta}{\partial t}$ which is assumed to be known, and applying Green's first identity, we obtain :

$$\begin{aligned} \delta\Omega(h,\eta) = & \int_R \left[-\frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial h}{\partial x_j} \right) \right] \tilde{h} dR - \int_{A_1} [h - H] K_{ij} \frac{\partial \tilde{h}}{\partial x_j} n_i dA + \int_{A_2} \left[K_{ij} \frac{\partial h}{\partial x_j} n_i + V \right] \tilde{h} dA \\ & - \int_F [h - \eta] K_{ij} \frac{\partial \tilde{h}}{\partial x_j} n_i dA + \int_F \left[K_{ij} \frac{\partial h}{\partial x_j} n_i - \left(I - S_y \frac{\partial \eta}{\partial t} \right) n_3 \right] \tilde{\eta} dA \\ & - \int_S [h - X_3] K_{ij} \frac{\partial \tilde{h}}{\partial x_j} n_i dA = 0 \end{aligned}$$

This method of not perturbing the term $\frac{\partial\eta}{\partial t}$ of the first variation enables us to derive a variational principle. Otherwise, the operator is not self adjoint and there does not exist a variational principle. With our assumption of $\frac{\partial\eta}{\partial t}$ known, we obtain an implicit expression that can be solved easily and, $\frac{\partial\eta}{\partial t}$ having been computed, we reiterate the computation : $\frac{\partial\eta}{\partial t}$ is considered as a known source term.

Furthermore, it is possible to use the Galerkin method instead of the Ritz method to solve this problem and the same result is obtained without any problem with the functional.

We can see on this first variation that our functional is correct, because, $\tilde{\eta}$ and \tilde{h} being arbitrary, it is necessary for all the equations written earlier, to be satisfied if we want $\delta\Omega$ to be zero.

For a given position of the free surface F , our mesh will be fixed and we can very easily assure with finite element the boundary conditions :

$$\begin{cases} h = H \text{ on } A_1 \\ h = X_3 \text{ on } S \\ h = \eta \text{ on } F \end{cases}$$

Furthermore, as $h = \eta$ on F , we can write $\frac{\partial \eta}{\partial t} = \frac{\partial h}{\partial t}$ on F and the functional is reduced to :

$$\Omega(h) = \int_R \left(\frac{1}{2} K_{ij} \frac{\partial h}{\partial x_j} \frac{\partial h}{\partial x_i} \right) dR + \int_{A_2} V h dA - \int_F h \left(I - S_y \frac{\partial h}{\partial t} \right) n_3 dA$$

Two-steps' iterative procedure

1/ On F and S , prescribed heads are given. Using the steady state equation, the flux ϕ is computed on F and S : we only need it on S .

2/ On S , the flux ϕ computed in step 1 is prescribed.

On F , a special boundary condition is given using the balance in the element.

The head is then determined.

Finite element equation

Substituting $h^N = h_n \xi_n$ and minimizing Ω with respect to h_n gives :

$$A_{nm} h_m + \sum_e \int_{F^e} \xi_n^e S_y \frac{\partial h}{\partial t} n_3 dA = Q_n + C_n$$

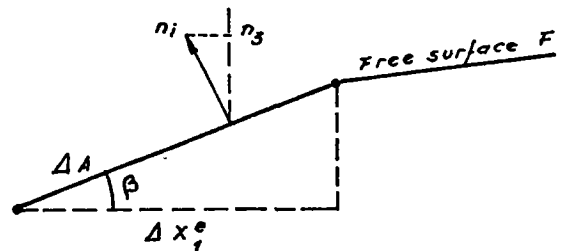
where :

$$C_n = \sum_e \int_{F^e} \xi_n^e I n_3 dA$$

Evaluation of C_n

a/ 2-dimensional problem

On the free surface F^e of an element e we have :



$$C_n^e = I n_3 \int_{F^e} \xi_n^e dA = I n_3 \frac{1}{2} \Delta A$$

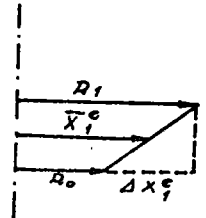
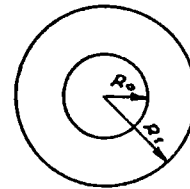
if ΔA is the length of the side along F of element e , as

$$n_3 = \cos \beta$$

$$\Delta A n_3 = \Delta X_1^e$$

and

$$C_n = \frac{1}{2} \sum_e I \Delta X_1^e$$



b) axi-symmetric problem

F becomes a surface and we integrate over the surface F :

$$C_n^e = I n_3 \int_{F^e} \xi_n^e dA = I n_3 \frac{1}{2} \Delta A$$

If one calculates directly the projection of the circular surface ΔA over the horizontal plane, one gets :

$$\begin{aligned} n_3 \Delta A &= \Pi \left(R_1^2 - R_0^2 \right) = 2\Pi \left(R_1 - R_0 \right) \left(\frac{R_1 + R_0}{2} \right) \\ &= 2\Pi \bar{X}_1^e \Delta X_1^e \end{aligned}$$

where R_1 and R_0 are the radii of the nodal points of the element, and \bar{X}_1^e the average value of these radii. Thus

$$C_n^e = \frac{1}{2} \sum_e I \Delta X_1^e \times 2\Pi \bar{X}_1^e$$

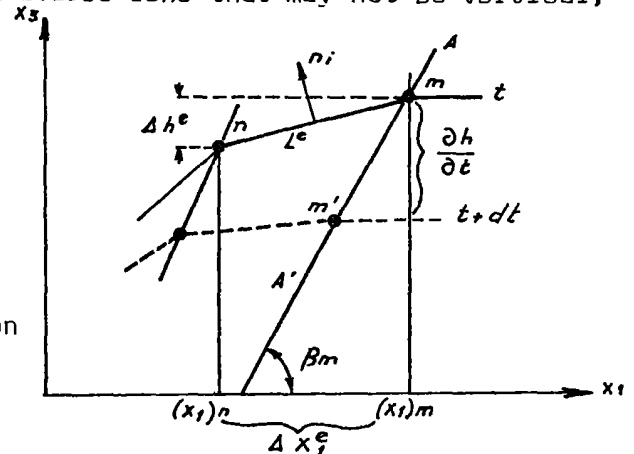
These two forms can be written

$$C_n = \frac{1}{2} \sum \alpha I \Delta X_1^e \quad \text{where} \quad \begin{cases} \alpha = 1 & \text{2-D problems} \\ \alpha = 2\Pi \bar{X}_1^e & \text{axi-symmetric problems} \end{cases}$$

Calculation of the displacement of the nodal points

The variation of the free surface with time, $\frac{\partial \eta}{\partial t}$ (or $\frac{\partial h}{\partial t}$ here) refers to the vertical movement of the points; in order to have the actual displacement of a node along a transverse line that may not be vertical, a correction must be made.

The nodal point m will move to m' along line AA' . This movement does not represent at all the one of a fluid particle. Along the free surface, the head $h = \eta$ is a function of time and X_1 only.



The displacement of m to m' along AA' induces a variation of head during the time step dt that can be calculated using the total derivative $\frac{dh}{dt}$. To get the partial derivative $\frac{\partial h}{\partial t}$ along the vertical (X_1 constant) we can write :

$$\frac{dh}{dt} = \frac{\partial h}{\partial X_1} \frac{dX_1}{dt} + \frac{\partial h}{\partial t}$$

As each segment of the free surface is a straight line and remains a straight line from t to $t + dt$, it is possible to calculate $\frac{dX_1}{dt}$ as a function of this expression itself taken only at the nodes on the free surface ; using the coordinate functions ξ^e :

$$\frac{dX_1}{dt} = \xi_p^e \left(\frac{dX_1}{dt} \right)_p$$

The same thing can be done for $\frac{dh}{dt}$:

$$\frac{dh}{dt} = \xi_m^e \left(\frac{dh}{dt} \right)_m$$

We then calculate $\frac{\partial h}{\partial t}$:

$$\frac{\partial h}{\partial t} = \xi_m^e \left(\frac{dh}{dt} \right)_m - \frac{\partial h}{\partial X_1} \xi_m^e \left(\frac{dX_1}{dt} \right)_m$$

Within element e, we can easily get $\frac{\partial h}{\partial X_1}$:

$$\frac{\partial h}{\partial X_1} = \frac{\Delta h^e}{\Delta X_1^e}$$

and

$$\left(\frac{dX_1}{dt}\right)_m = \left(\frac{dX_1}{dh} \frac{dh}{dt}\right)_m = \left(\frac{dh}{dt}\right)_m \cotg \beta_m$$

We finally get

$$\frac{\partial h}{\partial t} = \xi_m^e \left(\frac{dh}{dt}\right)_m \left(1 - \frac{\Delta h^e}{\Delta X_1^e} \cotg \beta_m\right)$$

Introducing this expression into the finite element equation :

$$A_{nm} h_m + \sum_e \int_{F_e} \xi_n^e S_y \frac{\partial h}{\partial t} n_3 dA = Q_n + C_n$$

we obtain

$$A_{nm} h_m + \sum_e \int_{F_e} \xi_n^e S_y \xi_m^e \left(\frac{dh}{dt}\right)_m \left(1 - \frac{\Delta h^e}{\Delta X_1^e} \cotg \beta_m\right) n_3 dA = Q_n + C_n$$

We can take $\left(\frac{dh}{dt}\right)_m$ out of the integral as is it is a constant in any element and we obtain, after calculation :

$$A_{nm} h_m + D_{nm} \left(\frac{dh}{dt}\right)_m = Q_n + C_n$$

where

$$A_{nm} = \sum_e \int_{R_e} K_{ij} \frac{\partial \xi_m^e}{\partial x_j} \frac{\partial \xi_n^e}{\partial x_i} dR$$

$$D_{nm} = \begin{cases} \sum_e \frac{\alpha}{3} S_y (\Delta X_1^e - \Delta h^e \cotg \beta_m) & , n = m \\ \sum_e \frac{\alpha}{6} S_y (\Delta X_1^e - \Delta h^e \cotg \beta_m) & , n \neq m \end{cases}$$

$$Q_n = - \sum_e \int_{A_2^e} V \xi_n^e dA$$

$$C_n = \frac{1}{2} \sum_e \alpha I \Delta X_1^e , \quad \alpha = \begin{cases} 1 & \text{planar flow} \\ \Pi [(X_1)_n + (X_1)_m] & \text{axi-symmetric} \end{cases}$$

D_{nm} and C_n are equal to zero everywhere except on the free surface.

Integration of this equation with respect to time

$$\text{Let } \Delta t = t^{k+1} - t^k \quad k = \text{number of time step}$$

We have 3 possibilities of approximating the derivative of h with respect to time :

a) Forward difference

$$A_{nm}^k h_m^k + D_{nm}^k \left(\frac{h_m^{k+1} - h_m^k}{\Delta t} \right) = Q_n^k + C_n^k$$

This is not stable for any Δt . Note that this method could be called "explicit" only if D_{nm} was a diagonal matrix.

b) Backward difference

$$A_{nm}^{k+1} h_m^{k+1} + D_{nm}^{k+1} \left(\frac{h_m^{k+1} - h_m^k}{\Delta t} \right) = Q_n^{k+1} + C_n^{k+1}$$

This expression is stable. It can be called "implicit".

c) Centred difference, or Crank - Nicholson formulation

$$\left\{ A_{nm}^{k+1} + \frac{D_{nm}^k}{\Delta t} + \frac{D_{nm}^{k+1}}{\Delta t} \right\} h_m^{k+1} = Q_n^k + Q_n^{k+1} + C_n^k + C_n^{k+1} - \left\{ A_{nm}^k - \frac{D_{nm}^k}{\Delta t} - \frac{D_{nm}^{k+1}}{\Delta t} \right\} h_m^k$$

This equation is programmed in Freesurf II.

Subscript k indicates that A, D, h... are taken at time t^k . These quantities are known and remain constant throughout the time step Δt .

Subscript k + 1 indicates values at time t^{k+1} : as they are ignored at the beginning of the resolution, an initial value will be estimated for the calculation of A, D and C and an iterative process will be generated :

$$\left\{ A_{nm}^j + \frac{D_{nm}}{\Delta t} + \frac{D_{nm}^j}{\Delta t} \right\} h_m^{j+1} = Q_n + Q_n^j + C_n + C_n^j - \left\{ A_{nm} - \frac{D_{nm}}{\Delta t} - \frac{D_{nm}^j}{\Delta t} \right\} h_m$$

In this notation, subscript j indicates the number of iteration applied to the evaluation of quantities at time k + 1. No subscript indicates known quantities at time k.

This iterative procedure has two steps, denoted $j + \frac{1}{2}$ and $J + 1$.

First step

Prescribed heads on boundaries F and S :

$$\begin{cases} h_m^{j+1/2} = \eta_m^j & \text{on F} \\ h_m^{j+1/2} = (X_3)_m^j & \text{on S} \end{cases}$$

one uses the equation written above to compute $h_m^{j+1/2}$ instead of h_m^{j+1} .

At the first iteration, an initial guess is made for the position of F and the length of S at time $t + \Delta t$.

When $h_m^{j+1/2}$ is computed, it is possible to determine the flow coming in or out of the system through the boundaries F and S :

$$Q_n^{j+1/2} = A_{nm}^j h_m^{j+1/2}$$

Second step

Prescribed Flux on boundaries F and S :

$$\left\{ \begin{array}{l} Q_S^{j+1/2} \text{ is set equal to the value computed at the first step on S.} \\ Q_F^{j+1/2} \text{ is set equal to zero if there is no infiltration, or equal to the} \\ \text{flow brought by infiltration, if there is any, on F.} \end{array} \right.$$

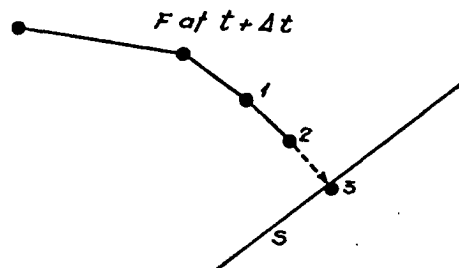
h_m^{j+1} is given by :

$$\left\{ A_{nm}^j + \frac{D_{nm}}{\Delta t} + \frac{D_{nm}^j}{\Delta t} \right\} h_m^{j+1} = Q_n + Q_n^{j+1/2} + C_n + C_n^j - \left\{ A_{nm} - \frac{D_{nm}}{\Delta t} - \frac{D_{nm}^j}{\Delta t} \right\} h_m$$

An error is then computed :

$$E = \max_F \left| \frac{h_m^{j+1} - h_m^j}{h_m^{j+1} - h_m} \right|$$

If $E > E_{\text{tolerable}}$, one shifts the free surface in order to achieve $h = \eta$ on F ; the intersection of F and S is determined in Freesurf II by extrapolating the direction of F towards S using the two adjacent nodes of F close to S.

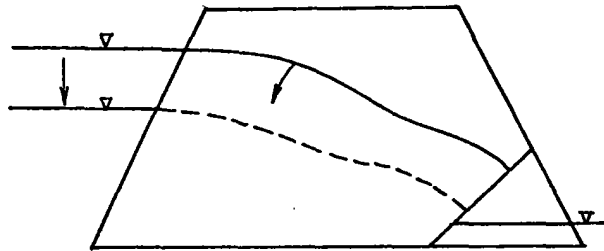


point 3 is extrapolated linearly from points 1 & 2

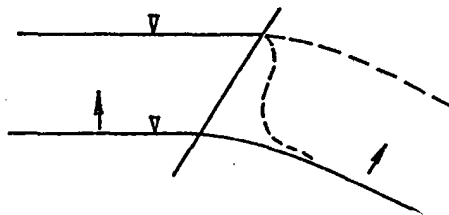
Moving the free surface modifies the matrices D_{nm}^j , C_n^j , A_{nm}^j and the processus continues.

Problems that can be solved by Free surf II

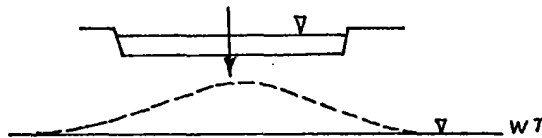
1) Dams.



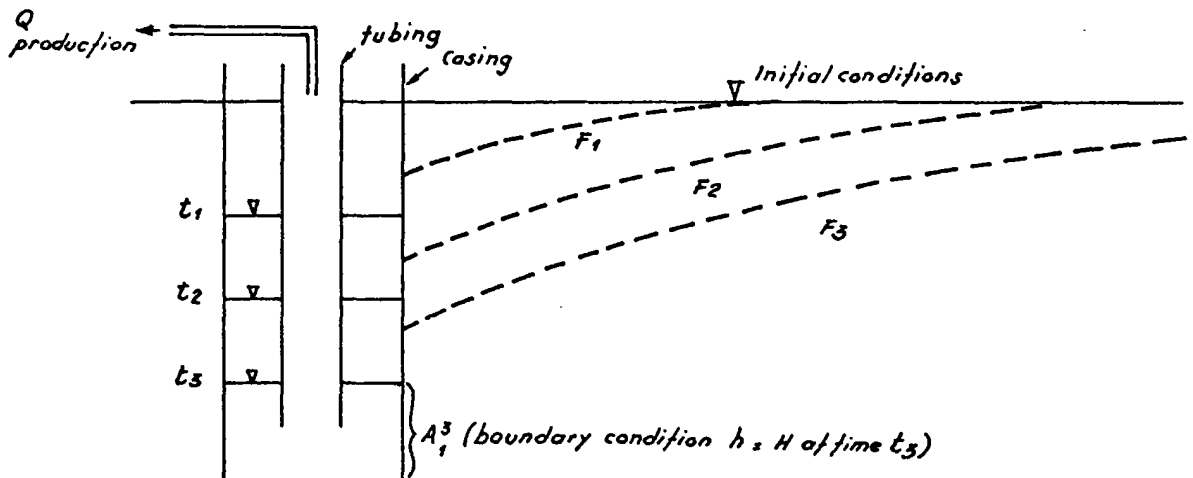
The level of water in the dam is supposed to be lowered, and not risen, otherwise the Free surface could be too tortuous and could intersect several times a transverse line, which, is not possible with this program :



2) Infiltration mounds.



3) Wells in free surface condition.



At prescribed production rate

Freesurf II takes into account the effect of the capacity of the well, using the inside diameter of the casing and the outside diameter of the tubing.

We can write :

$$Q \text{ production} = Q \text{ withdrawn from the well} + Q_{A_1+S}$$

(capacity effect) (withdrawn from aquifer)

We can assume that during time step Δt , there is a linear variation of Q_s :

$$Q \text{ production} = \frac{Q_p^k + Q_p^{k+1}}{2}$$

$$Q \text{ well effect} = \frac{Q_w^k + Q_w^{k+1}}{2}$$

$$Q \text{ aquifer} = \frac{Q_A^k + Q_A^{k+1}}{2}$$

If we define the volume produced during time step Δt ($V = Q\Delta t$) we can write :

$$\Delta V_p = \frac{\Delta t}{2} [Q_p^k + Q_p^{k+1}] = \frac{\Delta t}{2} [Q_A^k + Q_A^{k+1} + Q_w^k + Q_w^{k+1}]$$

$$\Delta V_w = \frac{\Delta t}{2} [Q_p^k + Q_p^{k+1}] - \frac{\Delta t}{2} [Q_A^k + Q_A^{k+1}]$$

$$\Delta V_w = \Delta L \cdot \Pi \cdot (r_c^2 - r_t^2) \quad \text{where } \Delta L \text{ is the lowering of the water level in the well.}$$

From this we get :

$$\Delta L = \frac{\Delta t}{2\Pi (r_c^2 - r_t^2)} \left[\underbrace{Q_p^k + Q_p^{k+1}}_{\text{known}} - \underbrace{Q_A^k - Q_A^{k+1}}_{\text{unknown}} \right]$$

It is necessary to know ΔL in order to fix the water level in the well and the prescribed head condition on A_1 . Therefore the resolution of this equation is introduced in the iterative procedure. If j is the number of iteration :

$$\Delta L^j = \frac{\Delta t}{2\pi (r_c^2 - r_t^2)} \left[Q_p + Q_p^j - Q_A - Q_A^j \right]$$

and

$$L^{j+1} = L - \Delta L^j \quad L \text{ being the level a time } t \text{ in the well.}$$

This permits to solve the problem of production in wells of large diameter (cf. Water Resources Research, June 71, p. 618).

Freesurf II can also solve the problem of prescribed head imposed in the well, instead of prescribed production rate.

VARIATIONAL PRINCIPLE

GENERAL PROBLEM

Let solve over a given domain the equation :

$$Ah = f$$

where A is an operator symmetrical and positive definite, f is a known function and h is an unknown function defined in the same domain.

We will prove that there is only one solution and that finding this solution is equivalent to determining the minimizing function of the functional :

$$\Omega(h) = \langle Ah, h \rangle - 2 \langle f, h \rangle$$

UNIQUENESS THEOREM

Assuming that : $h_1 \neq h_2$
we should have two solutions : $Ah_1 = Ah_2 = f$
let : $\Delta h = h_1 - h_2$
Then : $A(\Delta h) = f - f = 0$

A being a linear partial differential operator, the last equation implies :

$$\Delta h = 0 \quad \text{or} \quad h_1 = h_2$$

VARIATIONAL PRINCIPLE THEOREM

We will demonstrate now that h is a solution if and only if h minimizes the linear functional :

$$\Omega(h) = \langle Ah, h \rangle - 2 \langle f, h \rangle$$

We assume that A is real, positive definite, linear and self-adjoint.

1. For the first part of the proof we assume that h is the solution of the equation :

$$Ah = f$$

We now introduce some arbitrary function \tilde{h} having the same mathematical properties as h and satisfying the boundaries conditions. We replace h by $h + \tilde{h}$ in the functional :

$$\Omega(h + \tilde{h}) = \langle A(h + \tilde{h}), h + \tilde{h} \rangle - 2 \langle f, h + \tilde{h} \rangle$$

Ω and A being linear we can write :

$$\begin{aligned} \Omega(h + \tilde{h}) &= \langle Ah, h \rangle + \langle Ah, \tilde{h} \rangle + \langle A\tilde{h}, h \rangle + \langle A\tilde{h}, \tilde{h} \rangle - 2 \langle f, h \rangle - 2 \langle f, \tilde{h} \rangle \\ &= \Omega(h) + \langle Ah, \tilde{h} \rangle + \langle A\tilde{h}, h \rangle + \langle A\tilde{h}, \tilde{h} \rangle - 2 \langle f, \tilde{h} \rangle \end{aligned}$$

Because of the self-adjointness of A : $\langle A\tilde{h}, h \rangle = \langle Ah, \tilde{h} \rangle$

Then :

$$\Omega(h + \tilde{h}) = \Omega(h) + \langle A\tilde{h}, \tilde{h} \rangle + 2 \langle Ah - f, \tilde{h} \rangle$$

The last term of the right hand side of the equation vanishes because $Ah - f = 0$.

So that :

$$\Omega(h + \tilde{h}) = \Omega(h) + \langle A\tilde{h}, \tilde{h} \rangle$$

A is positive definite, then if \tilde{h} is non zero, the quantity $\langle A\tilde{h}, \tilde{h} \rangle$ is positive and we can write :

$$\Omega(h + \tilde{h}) > \Omega(h)$$

|| If h is a solution of the differential equation $Ah = f$, the functional of $h + \tilde{h}$ is always greater than the functional of h . Then h minimizes $\Omega(h)$.

2. For the second part of the proof we suppose that h minimizes $\Omega(h)$ so that :

$$\Omega(h + \Delta\lambda\tilde{h}) - \Omega(h) \geq 0$$

where $\Delta\lambda$ is a very small positive number.

By replacing h by $(h + \Delta\lambda\tilde{h})$ in our definition of the linear functional we get

$$\begin{aligned} \langle A(h + \Delta\lambda\tilde{h}), h + \Delta\lambda\tilde{h} \rangle - 2\langle f, h + \Delta\lambda\tilde{h} \rangle - \Omega(h) &= \langle Ah, h \rangle + \langle Ah, \Delta\lambda\tilde{h} \rangle + \langle A\Delta\lambda\tilde{h}, h \rangle \\ &+ \langle A\Delta\lambda\tilde{h}, \Delta\lambda\tilde{h} \rangle - 2\langle f, h \rangle - 2\langle f, \Delta\lambda\tilde{h} \rangle - \Omega(h) \end{aligned}$$

In this expression the terms 1, 5 and 7 vanish, so that by using the self-adjointness of A we finally get :

$$\Omega(h + \Delta\lambda\tilde{h}) - \Omega(h) = (\Delta\lambda)^2 \langle A\tilde{h}, \tilde{h} \rangle + 2(\Delta\lambda) \langle Ah - f, \tilde{h} \rangle$$

The first term of the right-hand side of this expression is always positive. $\Delta\lambda$ and \tilde{h} being arbitrary, the only way for this expression to be positive or equal to zero is to have :

$$\langle Ah - f, \tilde{h} \rangle = 0$$

This implies the following equation :

$$Ah - f = 0$$

|| So if h minimizes the functional $\Omega(h)$, then h is a solution of the differential equation :

$$Ah = f$$

- Why can we use the 1st variation test ?

We determine the first variation of $\Omega(h)$ through :

$$\delta\Omega(h) = \left. \frac{\partial}{\partial\lambda} \Omega(h + \lambda\tilde{h}) \right|_{\lambda=0}$$

By definition this is the following limit :

$$\begin{aligned} \delta\Omega(h) &= \lim_{\Delta\lambda \rightarrow 0} \frac{\Omega[h + (\lambda + \Delta\lambda)\tilde{h}] - \Omega(h + \lambda\tilde{h})}{\Delta\lambda} \Bigg|_{\lambda=0} \\ &= \lim_{\Delta\lambda \rightarrow 0} \frac{\Omega(h + \Delta\lambda\tilde{h}) - \Omega(h)}{\Delta\lambda} \end{aligned}$$

Using the second part of the previous theorem we can get the value of the limit :

$$\delta\Omega(h) = 2 \langle Ah - f, \tilde{h} \rangle$$

This is the proof that we can use this test. In clear :

- 1/ if h satisfies the partial differential equation then $\delta\Omega(h) = 0$
- 2/ if $\delta\Omega(h) = 0 \quad \forall \tilde{h}$, then $Ah = f$

EXISTENCE THEOREM

We have assumed that $\Omega(h)$ has a minimum and only one, if the operator A is positive bounded below. This means that for each h there exists some real number γ such that the inner product :

$$\langle Ah, h \rangle \geq \gamma^2 \|h\|^2$$

where $\|h\|^2$ is the norm defined as follows :

$$\|h\|^2 \equiv \langle h, h \rangle \quad \text{in a Hilbert's space}$$

This is a necessary condition but not sufficient.

Let us take a more general situation. What happens if :

$$Ah(x_i, t) = f(x_i, t) \quad \text{in our domain } R$$

with non-homogeneous boundary conditions :

$$G_n h(x_i, t) = g_n(x_i, t) \quad \text{on } \Gamma_n$$

A can be an integrodifferential operator, that is differential with respect to x_i , but integral with respect to t (convolution).

Because of the convolution and of the non-homogeneous boundary conditions the functional is given by :

$$\Omega(h) = \frac{1}{2} \langle Ah * h \rangle - \langle f * h \rangle + \sum_n I_{\Gamma_n}$$

The surface integral I_{Γ_n} , due to the non-homogeneous boundary condition, has two requirements :

$$a - \delta\Omega(h) = 0$$

$$b - G_n h = g_n \quad \text{all over } \Gamma_n$$

The principle of the calculus is :

1/ take $\Omega(h)$

2/ get $\delta\Omega(h)$

3/ search for I_{Γ_n} (not easy)

4/ verify that $G_n h = g_n$

Example 1

- Simple non-steady flow in a confined region :

$$1 * \frac{\partial}{\partial x_i} (K_{ij} \frac{\partial h}{\partial x_j}) = S_s (h - h_0)$$

with the boundary conditions :

- prescribed head on A_1 $h = H$

- prescribed flux per unit area on A_2 $K_{ij} \frac{\partial h}{\partial x_j} n_i = -V$

The problem is completely defined by this set of equations.

From the first differential equation we can get :

$$\text{an operator} \quad Ah = 1 * \frac{\partial}{\partial x_i} (K_{ij} \frac{\partial h}{\partial x_j}) - S_s h$$

$$\text{a function} \quad f = -S_s h_0$$

Let us check the self-adjointness of A. We will take any two functions u, v, satisfying zero boundary conditions. The question is :

$$\langle Au, v \rangle \stackrel{?}{=} \langle Av, u \rangle$$

Using the operator A as defined above we have on the domain R :

$$\langle Au * v \rangle \equiv \int_R \left[1 * \frac{\partial}{\partial x_i} (K_{ij} \frac{\partial u}{\partial x_j}) * v - S_s u * v \right] dR$$

Using now Green's first identity and remembering that the permeability tensor K_{ij} is symmetric everywhere in R, this identity becomes :

$$\langle Au * v \rangle \equiv \int_R \left[1 * K_{ij} \frac{\partial u}{\partial x_j} * \frac{\partial v}{\partial x_i} - S_s u * v \right] dR$$

K_{ij} and S_s , being not function of time, can be moved outside of the convolution so that :

$$\langle Au * v \rangle \equiv \int_R \left[1 * \frac{\partial}{\partial x_i} (K_{ij} \frac{\partial v}{\partial x_j}) * u - S_s v * u \right] dR$$

The right hand side of this equality is equal to $\langle Av * u \rangle$. This is the proof of the self-adjointness of A in our example.

We can now write the actual functional :

$$\Omega(h) = - \int_R \frac{1}{2} * K_{ij} \frac{\partial h}{\partial x_j} * \frac{\partial h}{\partial x_i} dR - \int_R S_s \left(\frac{1}{2} h - h_0 \right) * h dR + I_{A_1} + I_{A_2}$$

We have to set : $K_{ij} \frac{\partial h}{\partial x_j} n_i = -V$ on A_2 and the surface integral

I_{A_2} has to be equal to :

$$I_{A_2} = - \int_{A_2} 1 * V * h dA$$

And for I_{A_1} :

$$I_{A_1} = + \int_{A_1} 1 * (h - H) * K_{ij} \frac{\partial h}{\partial x_j} n_i dA$$

Example 2

- Variational principle in terms of head and velocity together.

In the region R the flow can be characterized by the following set of equations :

- continuity equation (combined with initial condition) $1 * \frac{\partial v_i}{\partial x_i} = - S_s (h - h_0)$

- Darcy's law $v_i = - K_{ij} \frac{\partial h}{\partial x_j}$

- Boundary conditions $h = H$ on A_1
 $v_i n_i = V$ on A_2

We will solve the continuity equation for h, assuming the velocity v as known, and the Darcy's law for v, assuming the head h as known. The problem is how to compute the functional Ω in terms of h and v_i together.

Looking for $\Omega(h)$, let us write the first differential equation :

$$A_1 h = f_1$$

assuming that : $A_1 h = - S_s h$

$$f_1 = 1 * \frac{\partial v_i}{\partial x_i} - S_s h_0$$

In terms of head the functional becomes :

$$\Omega(h) = - \int_R \left[S_s \left(\frac{1}{2} h - h_0 \right) * h + 1 * \frac{\partial v_i}{\partial x_i} * h \right] dR + I_1$$

Looking now for $\Omega(v_i)$, let us write the second differential equation :

$$A_2 v_i = f_2$$

assuming that : $A_2 v_i = - v_i$

$$f_2 = K_{ij} \frac{\partial h}{\partial x_j}$$

In terms of velocity the functional becomes :

$$\Omega(v_i) = - \int_R \left[\frac{1}{2} v_i * v_i + K_{ij} \frac{\partial h}{\partial x_j} * v_i \right] dR + I_2$$

The question is how to combine $\Omega(h)$ and $\Omega(v_i)$. For that we must somehow get $1 * \frac{\partial v_i}{\partial x_i} * h$ looking as $K_{ij} \frac{\partial h}{\partial x_j} * v_i$

Green's first identity leads to :

$$1 * \frac{\partial v_i}{\partial x_i} * h = - 1 * v_i * \frac{\partial h}{\partial x_i}$$

Using K_{ik}^{-1} defined by : $K_{ji} K_{ik}^{-1} = \delta_{jk}$ where δ_{jk} is Kronecker delta, and multiplying $\Omega(v_i)$ by $1 * K_{ik}^{-1}$, K_{ij} disappears and we get in $\Omega'(v_i)$ a similar expression to the above one got by applying Green's first identity on $\Omega(h)$.

By doing the union of $\Omega(h)$ and $\Omega'(v_i)$ we obtain the functional :

$$\Omega(h, v_i) = \Omega(h) \cup \Omega'(v_i)$$

or :

$$\Omega(h, v_i) = \int_R \left[1 * v_i * \frac{\partial h}{\partial x_i} + \frac{1}{2} * v_i * K_{ik}^{-1} v_k - S_s \left(\frac{1}{2} h - h_o \right) * h \right] dR + I$$

where I is a surface integral, very hard to find.

MATRIX SOLUTION OF THE PROBLEM (by G. GAMBOLATI)

It is possible to find the functional $\Omega(h, v_i)$ by using a matrix formulation of the basic equations :

$$\left. \begin{array}{l} \text{Continuity equation : } 1 * \frac{\partial v_i}{\partial x_i} = S_s (h - h_o) \\ \text{Darcy's law : } v_i = - K_{ij} \frac{\partial h}{\partial x_j} \end{array} \right\} \text{ on R}$$

This set of equations can be written :

$$- S_s h + 1 * \frac{\partial v_i}{\partial x_i} = - S_s h_o$$

$$v_i + K_{ij} \frac{\partial h}{\partial x_i} = o$$

or by matrix formulation :

$$\begin{bmatrix} - S_s & 1 * \frac{\partial}{\partial x_i} \\ \frac{\partial}{\partial x_i} & - K_{ij}^{-1} \end{bmatrix} \begin{bmatrix} h \\ v_i \end{bmatrix} = \begin{bmatrix} - S_s h_o \\ o \end{bmatrix}$$

① ② ③

The matrix ① corresponds to the operator A, the matrix ② to the vector ψ and the matrix ③ to the function f. From that formulation we can compute the following inner products :

$$\frac{1}{2} \langle A\psi * \psi \rangle = \frac{1}{2} \int_R \left[\left(- S_s h + 1 * \frac{\partial v_i}{\partial x_i} \right) * h + \left(\frac{\partial h}{\partial x_i} - K_{ij}^{-1} v_i \right) * v_i \right] dR$$

$$\langle f * \psi \rangle = - \int_R S_s h_o * h dR$$

The functional $\Omega(h, v_i)$ is then given by :

$$\Omega(h, v_i) = \Omega(\psi) = \frac{1}{2} \langle A\psi * \psi \rangle - \langle f * \psi \rangle$$

GALERKIN METHOD

The Galerkin method is applicable to both linear and non-linear problems, but it has the disadvantage that the boundary conditions cannot be embedded in the variational statement of the problem. We start with the following general set of equations :

$$Ah(x_i, t) = f(x_i, t) \quad \text{on } R$$

$$G_n h(x_i, t) = g_n(x_i, t) \quad \text{on } \Gamma_n$$

A is here just a differential operator. In general A is non linear and non self-adjoint. Some restrictions on the shape of A have been found by the previous researchers. But we use it now with no restriction and it works. We assume that :

$$h \approx h^N = h_n(t) \xi_n(x_i)$$

where $h_n(t)$ is the Galerkin coefficient and $\xi_n(x_i)$ the coordinate function.

The Galerkin criterion is based on the principle that the inner product of two orthogonal functions is equal to zero.

The problem is then to find the function h such that :

$$\langle Ah^N - f, \xi_n \rangle = 0$$

In this equation each one of Ah^N and f must be orthogonal to the coordinate function ξ_n . And finally we must have the following criterion :

$$\langle Ah_m \xi_m, \xi_n \rangle - \langle f, \xi_n \rangle = 0$$

Remark :

If we go back to the Ritz' method, we remember that :

$$\Omega(h) = \frac{1}{2} \langle Ah, h \rangle - \langle f, h \rangle$$

Then according to this equation :

$$\Omega(h) \approx \Omega(h^N) = \frac{1}{2} \langle Ah_m \xi_m, h_n \xi_n \rangle - \langle f, h_n \xi_n \rangle$$

And the first variation of $\Omega(h)$ will be equal to :

$$\delta_n \Omega(h^N) = \langle Ah_m \xi_m, \xi_n \rangle - \langle f, \xi_n \rangle$$

This first variation must be equal to zero. This result is exactly identical to the Galerkin's criterion. The only difference is that the Galerkin's method does not require the variational principle. We do not introduce the boundary conditions. This is hard in theory but easy in practice. The Galerkin's method is very convenient for Finite Element Method.

APPLICATION TO THE TRANSPORT OF SOLIDS

1. Treated by the Galerkin's method

- We will assume that we use an ideal tracer (some salt for instance), i.e. the specific weight of the water will be the same with or without salt.
- We assume steady flow conditions. The continuity equation will be :

$$\frac{\partial v_i}{\partial x_i} = 0$$

The velocity v_i is constant with time but can change from place to place. Then, let us take the following classical equation :

$$\frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c}{\partial x_j} \right) - v_i \frac{\partial c}{\partial x_i} = \phi \frac{\partial c}{\partial t}$$

in which D_{ij} is a tensor, called dispersion coefficient

$$\frac{\partial c}{\partial x_j} \text{ is the concentration gradient}$$

ϕ is the effective porosity

The boundary conditions will be :

$$C(x_i, 0) = C_0(x_i) \quad \text{on } R$$

where C_0 is a given function for starting.

$$c = C \text{ given} \quad \text{on } A_1$$

$$D_{ij} \frac{\partial c}{\partial x_j} n_i = - V(x_i, t) \text{ known on } A_2$$

where n_i is the normal to the boundary and V the flux due to dispersion not to velocity.

We also assume that the dispersion coefficient D_{ij} is symmetrical and positive :

$$D_{ij} = D_{ji} \geq 0$$

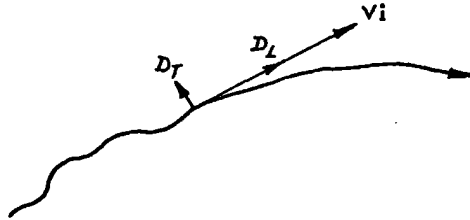
and that :

$$D_{ij} = f(x_i, v_i)$$

It is sometimes assumed that :

$$D_{ij} = \alpha_{ij} |v|$$

where α_{ij} is a constant value. But this assumption is not always true. We cannot neglect anisotropy with respect to D_{ij} :



The figure above shows the longitudinal dispersion D_L and the transverse dispersion D_T .

Applying the operator A to the concentration c we may write :

$$Ac = - \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c}{\partial x_j} \right) + v_i \frac{\partial c}{\partial x_i} + \phi \frac{\partial c}{\partial t}$$

This entire expression is not self-adjointed, so we cannot develop a variational principle and then we use the Galerkin's method.

We can now go directly to the Finite Element Method by writing the approximation :

$$c^N = c_n \xi_n$$

where ξ_n is still the coordinate function.

The summation within each element gives :

$$\sum_e \int_{R^e} \left[\frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial \xi_m^e}{\partial x_j} \right) c_m \xi_n^e - v_i \frac{\partial \xi_m^e}{\partial x_i} c_m \xi_n^e - \phi \frac{\partial c}{\partial t} \xi_n^e \right] dR$$

and this expression must be equal to zero.

We let intact $\frac{\partial c}{\partial t}$ because we want to define at nodal point n :

$$\left(\frac{\partial c}{\partial t} \right)_n = \frac{\sum_e \int_{R^e} \phi \frac{\partial c}{\partial t} \xi_n^e dR}{\sum_e \int_{R^e} \phi \xi_n^e dR}$$

Then we can write :

$$\left(AA_{nm} + B_{nm} \right) C_m + D_n \left(\frac{\partial c}{\partial t} \right)_n = Q_n$$

where :

$$AA_{nm} = \sum_e \int_{Re} D_{ij} \frac{\partial \xi_n^e}{\partial x_j} \frac{\partial \xi_m^e}{\partial x_i} dR$$

$$B_{nm} = \sum_e \int_{Re} v_i \xi_n^e \frac{\partial \xi_m^e}{\partial x_i} dR$$

$$D_n = \sum_e \int_{Re} \phi \xi_n^e dR$$

$$Q_n = - \sum_e \int_{A_e} V \xi_n^e dA$$

In these expressions v_i and D_{ij} are taken constant inside each element.

Remark :

If v_i and D_{ij} vary linearly^{within} each element instead of being constant, we must change them into a linear approximation :

$$D_{ij} = (D_{ij})_m^e \xi_m^e$$

$$v_i = (v_i)_m^e \xi_m^e$$

2. Treated by the Ritz' method

Using the operator A with respect to the concentration c we define :

$$Ac = - \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial c}{\partial x_j} \right)$$

and the function :

$$f = - v_i \frac{\partial c}{\partial x_i} - \phi \frac{\partial c}{\partial t}$$

This is one way to use the Ritz method. There is an other one used by GUYMON described below. We had :

$$Ac = 0$$

Then we take a weight function $g(x_i)$ and we write :

$$1 * \frac{\partial}{\partial x_i} \left[g(x_i) D_{ij} \frac{\partial c}{\partial x_j} \right] = g(x_i) \Phi (c - c_0)$$

By doing so we assume that there exists a function g . We also assume that :

$$D_{ij}, v_i \neq f(x_i)$$

Therefore, assuming a constant velocity ~~with~~ in each element and using :

$$- D_{ij} \frac{\partial g}{\partial x_j} = gv_i$$

we should get the same result as before.

To solve this equation we may write :

$$g = e^{-b_k X_k}$$

where b_k are solutions of :

$$D_{ij} b_j = v_i \quad i = 1, 2, 3$$

If solved in 2-dimensions we can see that b_k are constant values :

$$b_1 = \frac{v_1 D_{22} - v_2 D_{12}}{D_{11} D_{22} - D_{12} D_{21}}$$

$$b_2 = \frac{v_2 D_{11} - v_1 D_{21}}{D_{11} D_{22} - D_{12} D_{21}}$$

The transformed operator being self-adjoint the functional $\Omega(c)$ is given by :

$$\begin{aligned} \Omega(c) = & \int_R \left[\frac{1}{2} * D_{ij} \frac{\partial c}{\partial x_j} * \frac{\partial c}{\partial x_i} + c * \left(\frac{1}{2} c - c_0 \right) \right] e^{-b_k X_k} dR \\ & - \int_{A_1} 1 * (c - C) * D_{ij} \frac{\partial c}{\partial x_j} n_i e^{-b_k X_k} dA_1 + \int_{A_2} 1 * V * c e^{-b_k X_k} dA_2 \end{aligned}$$

Guymon uses an intermediate function given by :

$$\eta^N = C^N e^{-\frac{1}{2} \sum_k X_k^2}$$

FRACTURE FLOW

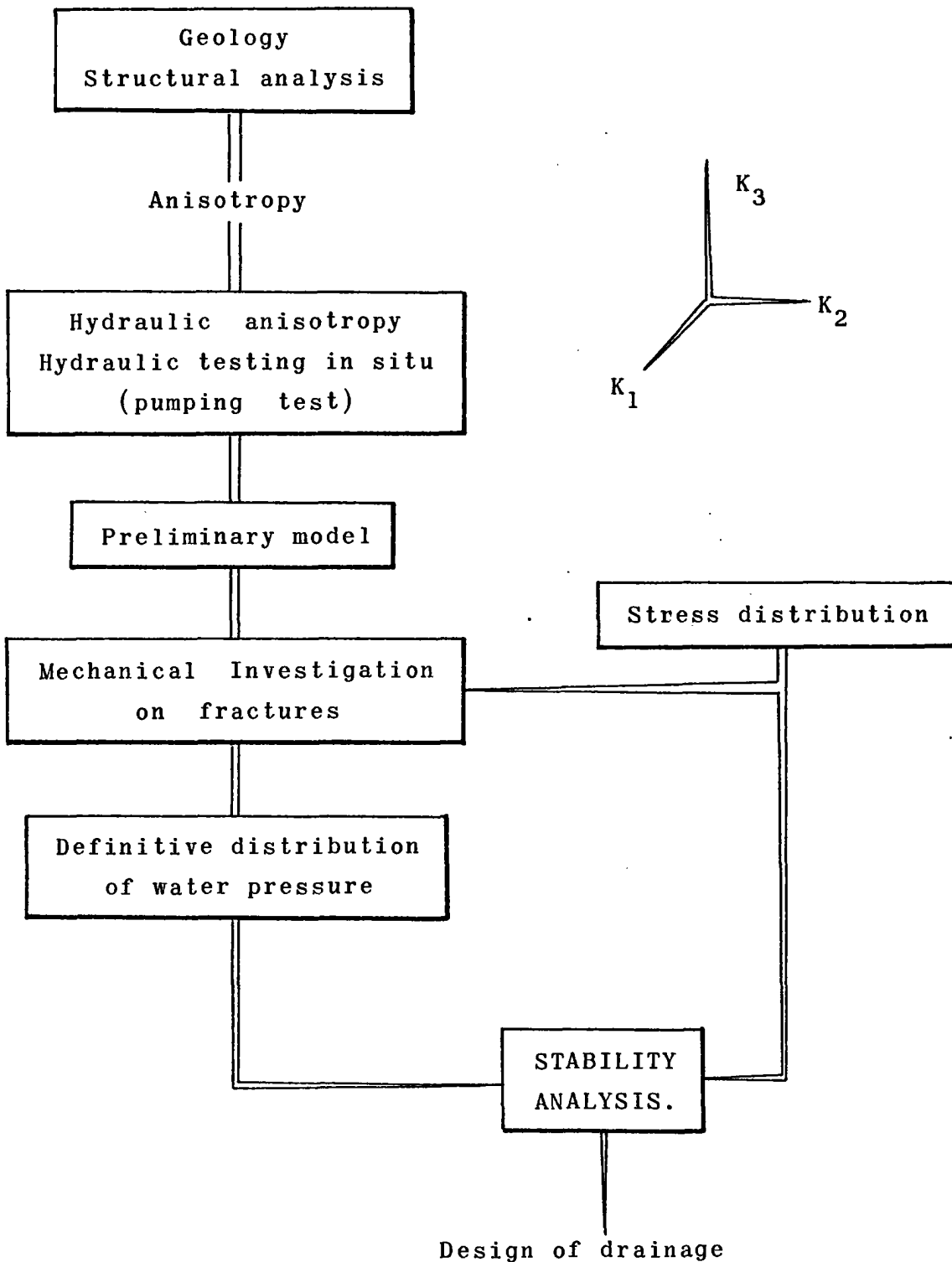
In general, there is a complicated interaction in a fractured rock mass between the forces exerted by the fluids and those exerted by body forces and boundary loads.

- From the fluid flow standpoint, it is very important and more realistic to consider individual fracture characteristics in analyzing flow through jointed rocks. This consideration leads to various flow laws depending upon the Reynolds Number and the relative roughness of the fracture (Louis, 1969). It is necessary also to consider the deformability of the fracture due to existing forces, i. e. forces due to both fluid pressure and rock stresses and not only to fluid pressure.
- From the standpoint of structural analysis of engineering works, it is possible now to take into account the behavior of the joints or the fractures governing the stability of the rock masses (Goodman, Taylor and Brekke, 1968 - Mahtab, 1969 - Dubois and Goodman, 1971). When water is flowing through the fracture, forces due to water pressure must be coupled to body forces and eventually to boundary loads (Noorishad, Witherspoon and Brekke, 1971).

Fracture flow analysis is very important in a wide field of application :

- underground openings
- dam foundations
- reservoir flow
- open pit-mines
- geothermal
- earthquake modification
- underground explosives.

The general scheme of a stability analysis is given by Louis (1972) :



- General approach

The method used by Noorishad, Witherspoon and Brekke (1971) employs two finite element techniques and a converging iteration process. The program is restricted to the two-dimensional case, but can be extended to ^{the} three-dimensional one. The procedure is shown in the form of a flow chart in figure 1.

First the Stress program is used to determine the effect of the structure (dam, tunnel, etc...) on the rock mass. This analysis changes the size distribution of the fracture apertures. Then the flow program is used to determine a first approximation for pressure P_I at every point within the fractures.

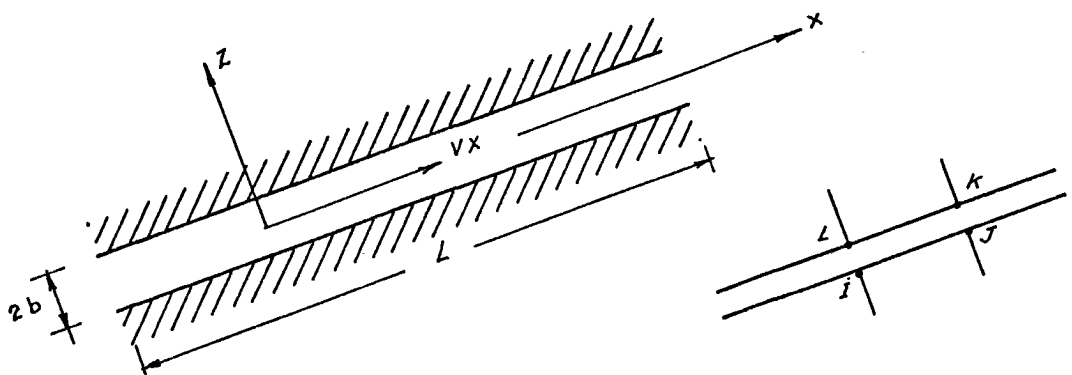
In a second step the stress analysis is repeated using both the effects of the structure and the fluid pressure P_I , giving a new modification of the apertures. By making a second flow analysis we get a second approximation for pressure P_{II} .

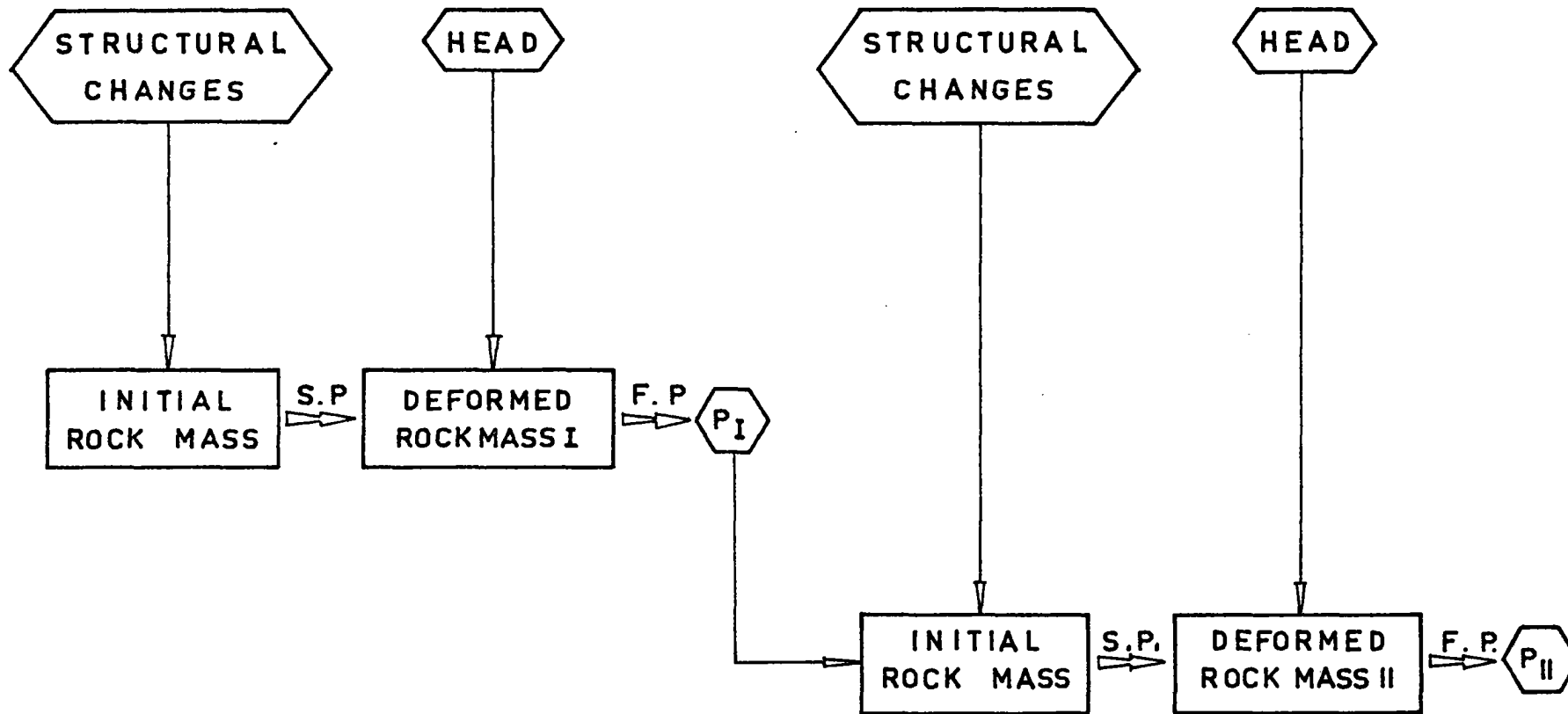
If $|P_{II} - P_I|$ is unacceptable, then the process is repeated until $|P_i - P_{i-1}|$ reaches a value less than some arbitrary chosen limit.

The rate of convergence to an acceptable solution was found to be quite rapid in all of the particular cases that were studied (Fig. 2).

- Fluid flow analysis

In the following discussion only steady state flow will be considered. A joint will be simulated by two parallel planes :





S P = Stress Program
 F P = Flow Program

FIG. 1 - FLOW CHART FOR ITERATION PROCESS

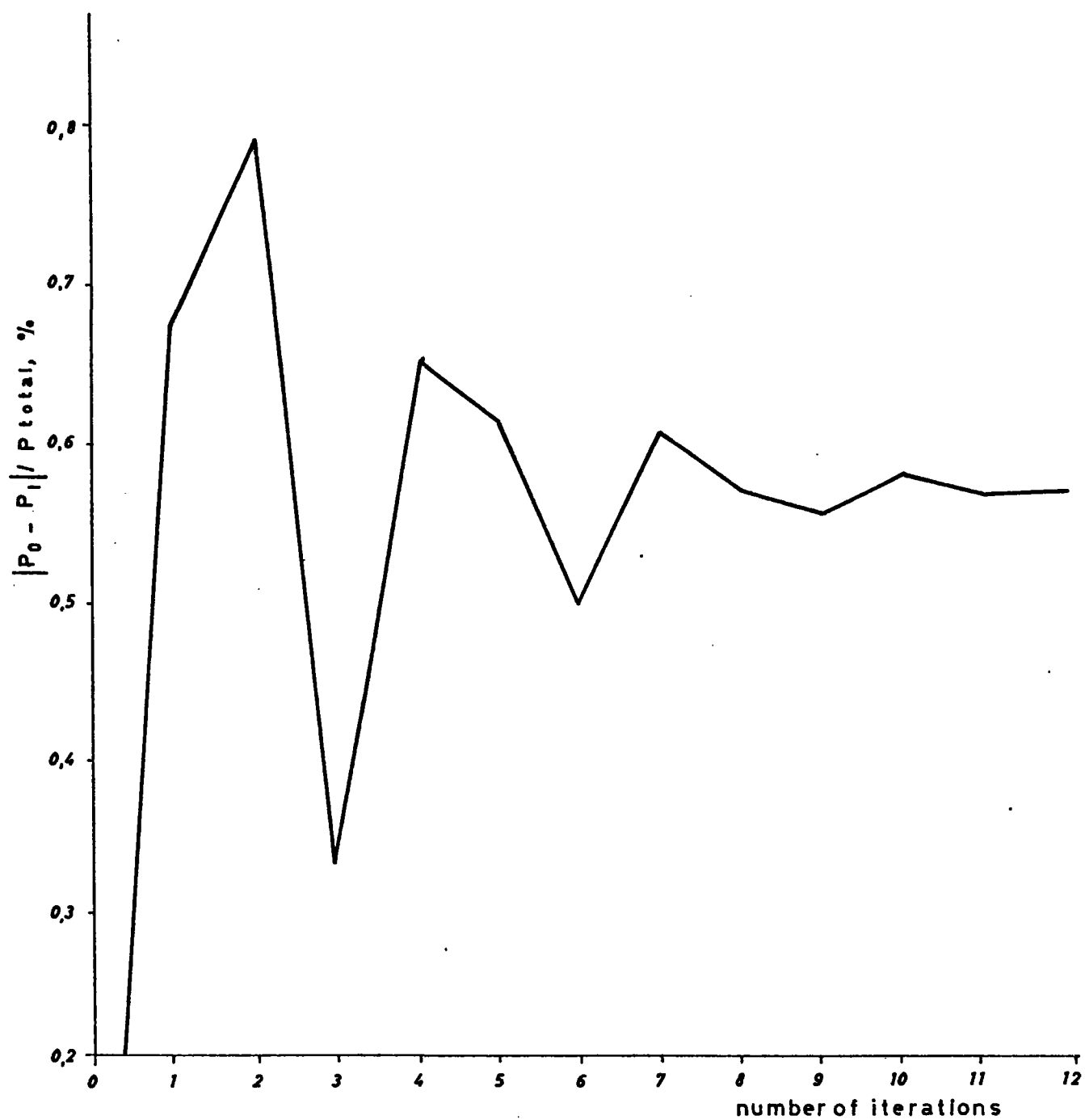


FIG. 2 - CONVERGENCE CHARACTERISTICS FOR TEST PROBLEM.

From the Finite Element point of view a joint is considered as a line element : the nodal points I and L, or J and K, have the same coordinates.

Steady state flow of an incompressible fluid through a single fracture or joint is governed by the following differential equation :

$$\frac{\partial}{\partial l} \left(k_p \frac{\partial h}{\partial l} \right) = 0$$

where k_p is called "area permeability" and is defined by :

$$k_p \equiv (2b.1) K_p$$

K_p being the fracture permeability depending upon the mass density of the fluid, the viscosity of the fluid and the aperture of the fracture.

l is a variable length along the fracture.

Solving the previous differential equation is a similar problem to that of finding a function h that satisfies the boundary conditions and minimizes the following functional :

$$\Omega(h) = \frac{1}{2} \int k_p \left(\frac{\partial h}{\partial l} \right)^2 dl$$

For the entire system and in the general case where flow quantities have been prescribed at some boundary, the functional can be written :

$$\Omega(h) = \sum_{m=1}^M \frac{1}{2} \int_{L^m} k_p^m \left(\frac{\partial h}{\partial l} \right)^2 dl + \sum_{m=1}^N \{q^m\}^T \{h^m\}$$

where M = number of elements

L^m = length of m -th segment in a network of M elements

N = number of boundary elements where q is prescribed.

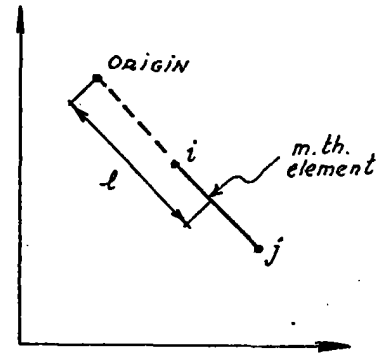
It can be proved that this functional is minimized by a particular function h for any joint element either inside the network or at the boundaries where head or flow are prescribed. We need now to find the minimizing function and for that purpose it is only necessary to demonstrate the procedure for a typical element m .

First we compute :

$$\frac{\partial \Omega^m(h)}{\partial h^m} = \left\{ \begin{array}{c} \frac{\partial \Omega^m(h)}{\partial h_i} \\ \frac{\partial \Omega^m(h)}{\partial h_j} \end{array} \right\}$$

where :

$$\frac{\partial \Omega^m(h)}{\partial h_i} = \int_{L^m} k_p^m \left(\frac{\partial h}{\partial l} \right) \frac{\partial}{\partial h_i} \left(\frac{\partial h}{\partial l} \right) dl + q_i$$



Remember that we consider a line element, along which h varies linearly :

$$h = c + dl$$

Since

$$\frac{\partial h}{\partial l} = \begin{bmatrix} \frac{\partial N_i}{\partial l} & \frac{\partial N_j}{\partial l} \end{bmatrix} \begin{Bmatrix} h_i \\ h_j \end{Bmatrix} = \begin{bmatrix} -\frac{1}{L^m} & \frac{1}{L^m} \end{bmatrix} \begin{Bmatrix} h_i \\ h_j \end{Bmatrix}$$

where :

$$N_i = \frac{l_j - l}{l_j - l_i} = \frac{l_j - l}{L^m}$$

$$N_j = \frac{l - l_i}{l_j - l_i} = \frac{l - l_i}{L^m}$$

we can write :

$$\frac{\partial \Omega^m(h)}{\partial h^m} = \begin{bmatrix} k_p^m / L^m & -k_p^m / L^m \\ -k_p^m / L^m & k_p^m / L^m \end{bmatrix} \begin{Bmatrix} h_i \\ h_j \end{Bmatrix} + \begin{Bmatrix} q_i \\ q_j \end{Bmatrix}$$

or simply :

$$\frac{\partial \Omega^m(h)}{\partial h^m} = [k_f] \{ h^m \} + \{ q^m \}$$

over the entire domain we get :

$$\frac{\partial \Omega(h)}{\partial h_i} = \sum_{m=1}^M \frac{\partial \Omega^m(h)}{\partial h_i} = 0$$

which can be written for all elements and nodal points :

$$\frac{\partial \Omega(h)}{\partial h_i} = \sum_{n=1}^M \sum_{i=1}^N (k_f)_{im} h_m + q_i = 0$$

Finally :

$$[K_f] \{h\} - \{Q\} = 0$$

where $[K_f]$ is the flow conductivity matrix.

- Flow forces within fractures

Knowing the distribution of pressures at every point within fractures, it is now possible to calculate the equivalent nodal point forces of these fluid pressure, that will be used later in the stress analysis.

Two kinds of forces are involved :

- normal forces
- tangential forces.

The fluid pressure acting in a fracture is shown on figure 4. In spite of the use of line element it is of course necessary to identify both sides of the fracture with the four nodal points i , j , k and l . The pressure P_i will be the same at both points i and l , and P_j at points j and k .

Normal forces :

From the laws of static equilibrium we can write :

$$\left\{ \begin{array}{c} F_{ix} \\ F_{iz} \\ F_{jx} \\ F_{jz} \\ F_{kx} \\ F_{kz} \\ F_{lx} \\ F_{lz} \end{array} \right\} = \frac{1}{6} \left[\begin{array}{cc} 2z_{ji} & z_{ji} \\ 2x_{ij} & x_{ij} \\ z_{ji} & 2z_{ji} \\ x_{ij} & 2x_{ij} \\ z_{lk} & 2z_{lk} \\ x_{kl} & 2x_{kl} \\ 2z_{lk} & z_{lk} \\ 2x_{kl} & x_{kl} \end{array} \right] \left\{ \begin{array}{c} P_i \\ P_j \end{array} \right\}$$

where F_{ix} and F_{iz} are the components of the equivalent point load at nodal point i and where :

$$z_{ji} = z_j - z_i$$

$$x_{ij} = x_i - x_j$$

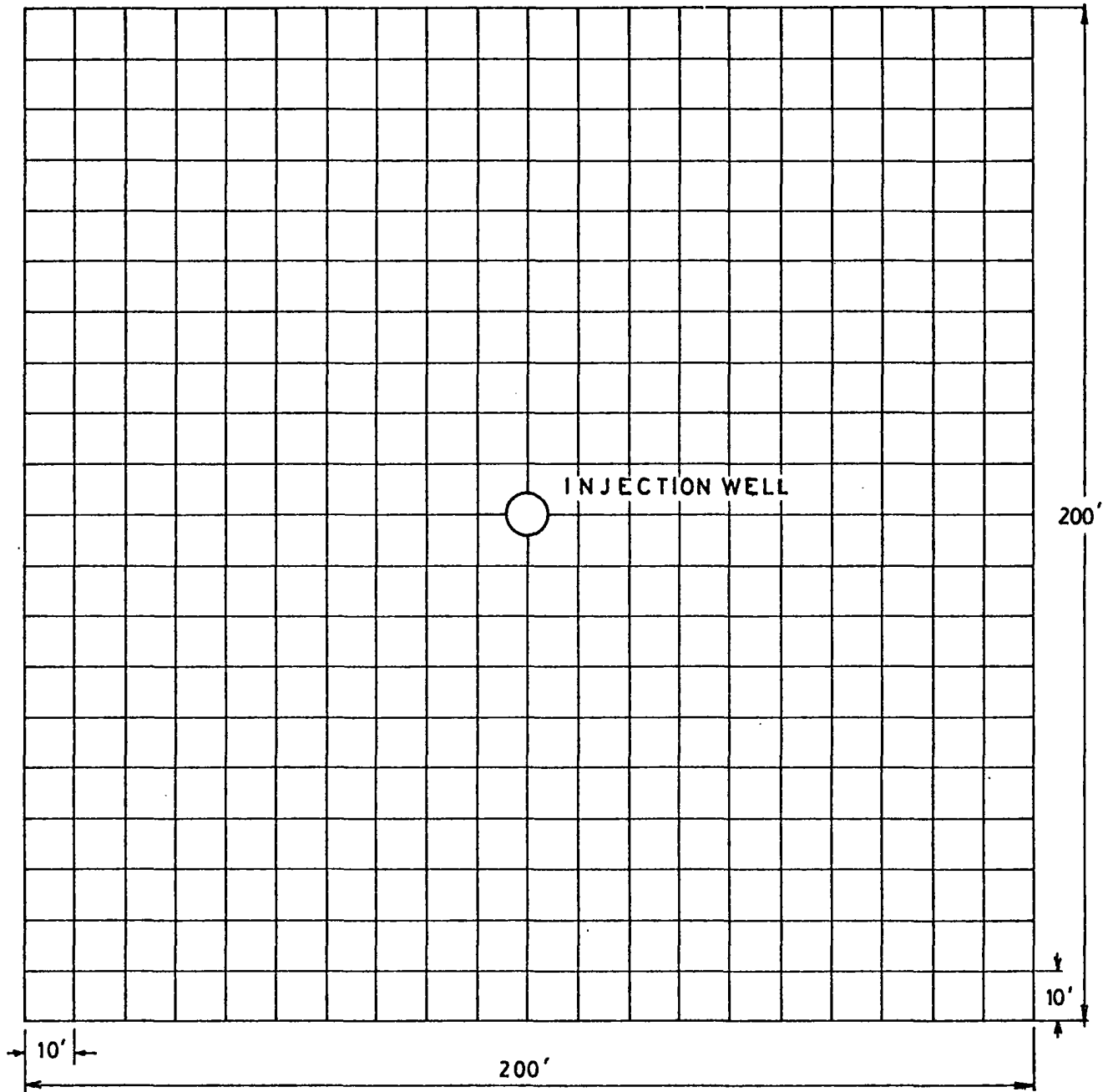


FIG. 3 - MODEL OF SQUARE FRACTURE SYSTEM

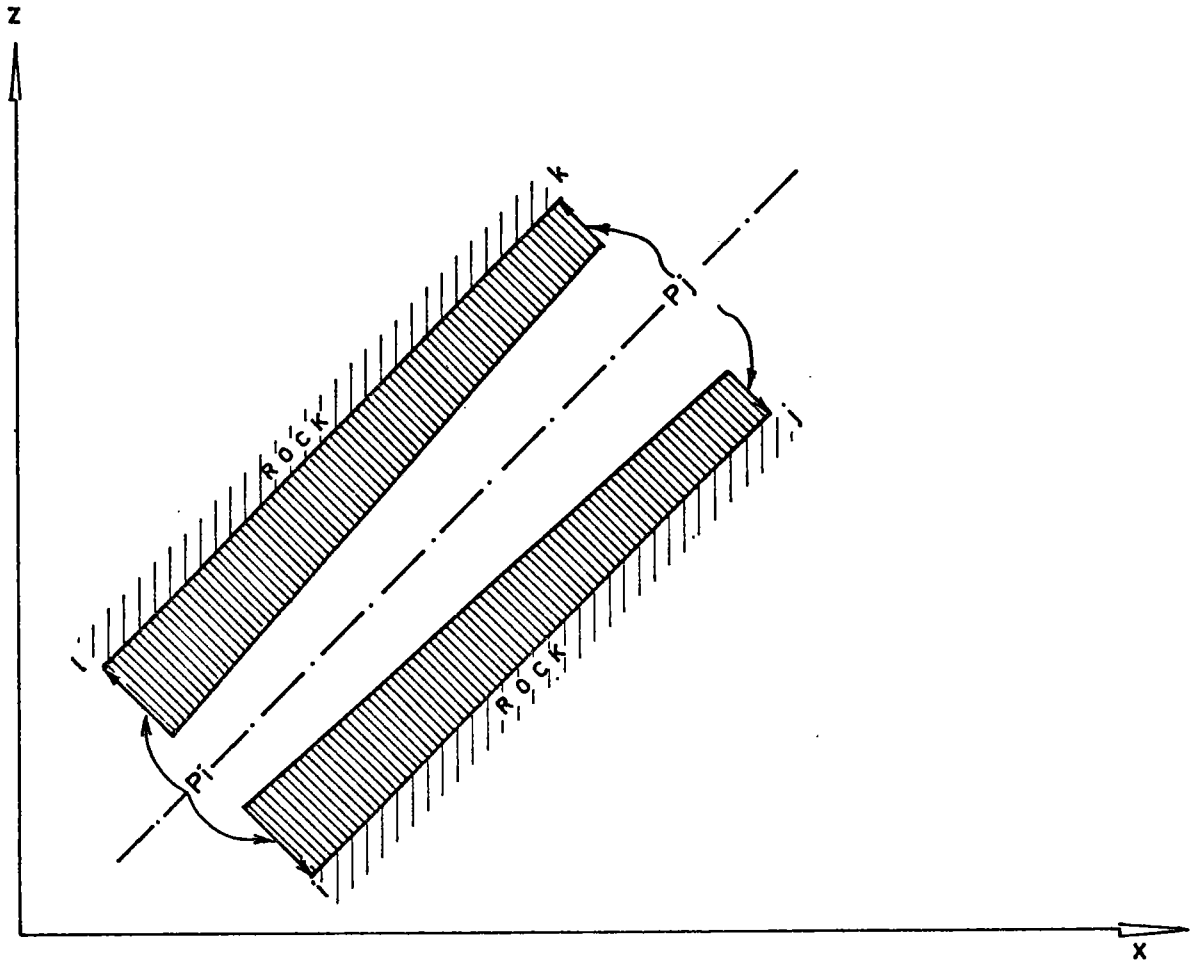


FIG. 4 - FLUID PRESSURE IN A FRACTURE

Tangential forces :

They are usually so small that they can be neglected.

- Stress and strain analysis

This analysis is based on an energy approach. The principle of minimum potential energy can give us a variational principle.

Let us write the total potential energy of our system :

$$W = \sum_{m=1}^M W^m - \{R\}^T \{\delta\}$$

where W^m is the potential energy contained within the element m , $\{R\}$ is the potential energy of boundary loads at the nodes, and $\{\delta\}$ is the displacement of the nodal points.

For each element :

$$W^m = \int_{V^m} \left[\frac{1}{2} \{\epsilon^m\}^T [c] \{\epsilon^m\} - \{\epsilon^m\}^T \{\sigma_0^m\} - \{G^m\}^T \{f^m\} \right] dV - \int_{S^m} \{P^m\}^T \{f^m\} dS$$

where :

$\{\epsilon^m\}$ is the strain vector and is equal to : $[B^m] \{\delta^m\}$ with $[B^m]$ = element deformation matrix.

$[c]$ is the elasticity matrix depending upon the elasticity modulus E and the Poisson ratio ν

$\{\sigma_0^m\}$ is the initial stress vector

$\{G^m\}$ are the distributed boundary loads

$\{f^m\}$ is the displacement vector within the elements and is equal to : $\{f^m\} = [N^m] \{\delta^m\}$

with N^m = a function of element coordinates

δ^m = element nodal point displacement vector

$\{P^m\}$ is the boundary distributed force vector

Substituting values of $\{f^m\}$ and $\{\epsilon^m\}$ we get :

$$\begin{aligned}
 W^m &= \frac{1}{2} \int_{V^m} \{\delta^m\}^T [B^m]^T [C] [B^m] \{\delta^m\} dV \\
 &- \int_{V^m} \left[\{\delta^m\}^T [B^m]^T \{\sigma_o^m\} - \{G^m\}^T [N^m] \{\delta^m\} \right] dV \\
 &- \int_{S^m} \{P^m\}^T [N^m] \{\delta^m\} dS
 \end{aligned}$$

As for flow problem we are looking for a function, in this case $\{\delta\}$, minimizing the functional W :

$$\frac{\partial W}{\partial \{\delta_i\}} = \sum_{m=1}^M \frac{\partial W^m}{\partial \{\delta_i\}} - \{R_i\} = 0$$

The operation results in :

$$\begin{aligned}
 &\sum_{m=1}^M \int_{V^m} [B^m]^T [C] [B^m] \{\delta^m\} dV \\
 &- \sum_{m=1}^M \left[\int_{V^m} \left([B^m]^T \{\sigma_o^m\} - \{G^m\}^T [N^m] \right) dV - \int_{S^m} \{P^m\}^T [N^m] dS \right] - \{R_i\} = 0
 \end{aligned}$$

or more simply :

$$\sum_{m=1}^M [K_c^m] \{\delta^m\} - \sum_{m=1}^M \{F^m\} = 0$$

where $[K_c^m]$ is the element stiffness matrix of the continuum and

$\{F^m\}$ is the nodal force vector of the element including G , P and R .

Summed over the entire system this equation can be written :

$$[K_c] \{\delta\} - \{F\} = 0$$

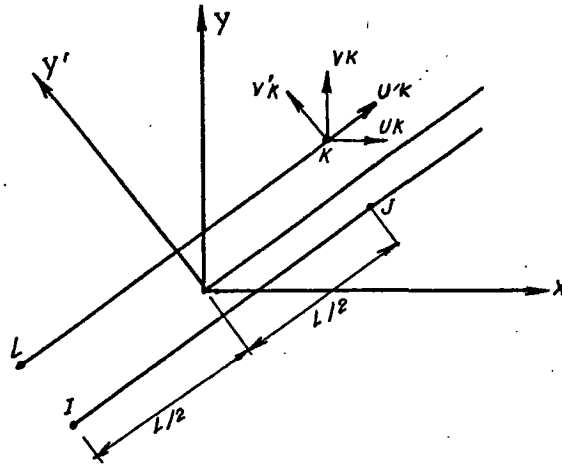
This equation is called the equilibrium equation and is a set of linear simultaneous algebraic equations that can be solved for nodal point displacements $\{\delta\}$.

Before coupling flow and stress analysis, it is necessary to have some knowledge of the joint behavior in the nature. This behavior may be summarized as follows :

- . a joint has no resistance to tension in the normal direction
- . a joint has resistance to compression in the normal direction
- . at low normal pressures, the shear strength is mainly cohesive.

A hypothetical stress-displacement relationship is shown in Figure 5.

Let represent a joint as follows : (after Goodman, Taylor and Brekke, 1968)



X and Y are the global coordinates and X' and Y' are the local coordinates.

U'_K is the shear displacement in local coordinates

V'_K is the normal displacement in local coordinates.

U_K and V_K are the nodal K displacements in global coordinates.

In the joint element of length L we have the following potential energy :

$$W = \int_{-\frac{L}{2}}^{\frac{L}{2}} \frac{1}{2} \{w'\}^T \{F'\} dx'$$

where $\{w'\}$ is the relative displacement between the top (say L, K) and the bottom (say I, J) sides of the joint, under the influence of an applied force F' per unit length.

Let $[K'_j]$ be the joint element stiffness matrix in the local coordinates :

$$[K'_j] = \int_{-\frac{L}{2}}^{\frac{L}{2}} [D] [C_j] [D] dx'$$

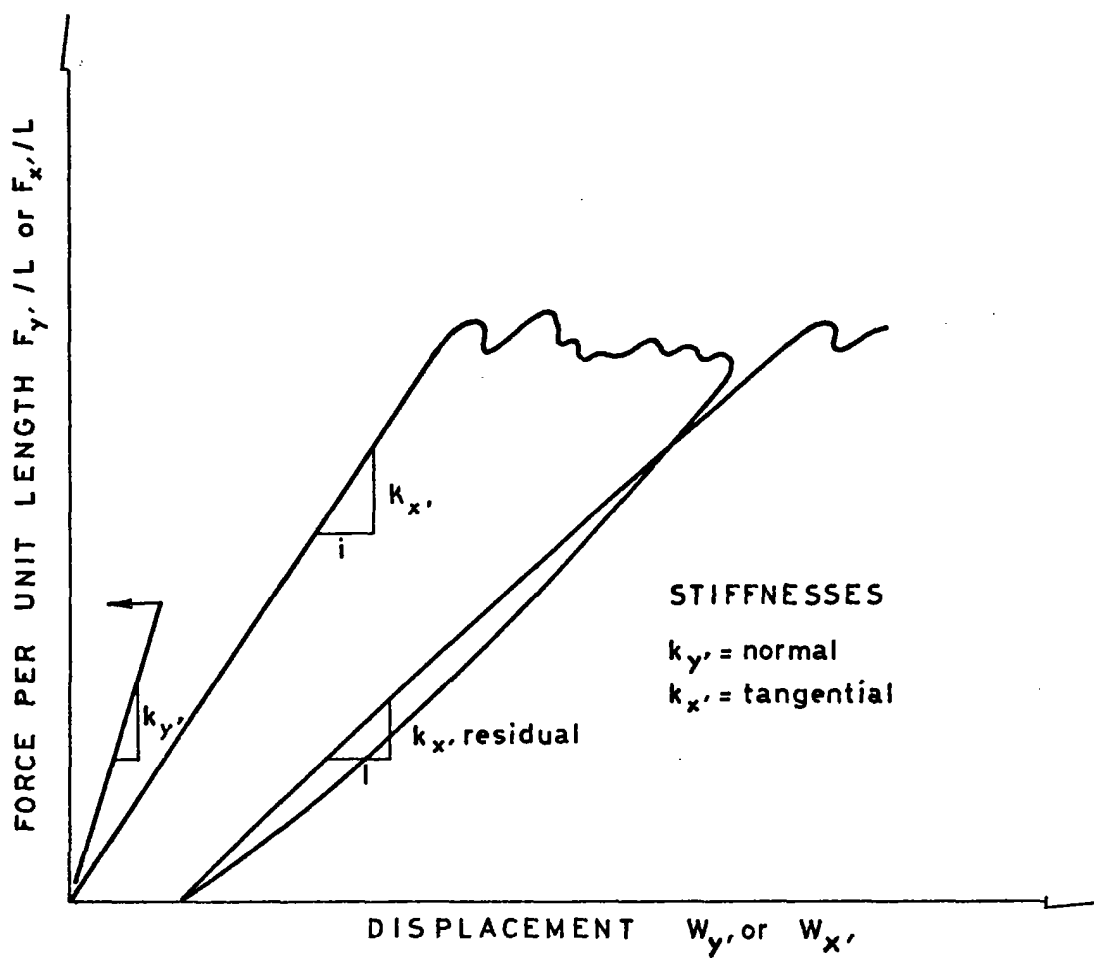


FIG. 5 - HYPOTHETICAL STRESS DISPLACEMENT RELATIONSHIP FOR A JOINT (AFTER GOODMAN ET AL., 1968).

where :

$[D]$ = displacement function relating the relative displacement $\{w'\}$ to nodal point displacement $\{\delta'\}$

$$[C_j] = \text{joint element moduli matrix} = \begin{bmatrix} k_x & 0 \\ 0 & k_y \end{bmatrix}$$

k_x , and k_y , being the normal and the shear stiffness of the joint in local coordinates.

The transformation from local to global coordinates gives us the joint stiffness :

$$[K_j] = [H]^T [K'_j] [H]$$

where $[H]$ is the transformation matrix.

Finally in the mathematical formulation used for the stress analysis, the total stiffness matrix $[K]$ of the system analyzed is the proper combination of the continuum elements stiffness matrix $[K_c]$ and the joint elements stiffness matrix $[K_j]$.

So the mechanical properties of both continuum and joint elements can be properly represented by :

$$[K] \{\delta\} - \{F\} = 0$$

- Stress - Flow analysis

The coupling between flow pressure and rock stresses must be satisfied by an iterative procedure that assures compatibility between rock stresses and fluid pressures. The two basic equations we have derived earlier are :

$$\begin{array}{ll} \text{for Flow} & [K_f] \{h\} - \{Q\} = 0 \\ \text{for Stress} & [K] \{\delta\} - \{F\} = 0 \end{array}$$

or more explicitly :

$$\begin{array}{ll} \frac{1}{\gamma} [K_f(\delta)] \{P\} - \{Q\} = 0 & \text{with } K_f(\delta) \left| \begin{array}{l} = 0 \\ \delta = 0 \end{array} \right. \\ [K] \{\delta\} - \{F(P)\} = 0 & \text{with } F(P) \left| \begin{array}{l} = 0 \\ P = 0 \end{array} \right. \end{array}$$

$K_f(\delta)$ indicates that flow conductivity is dependent on the joint deformations.

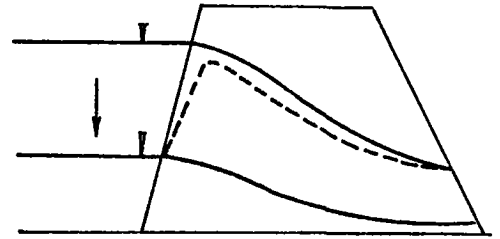
$\{P\}$ is the equivalent pressure of the net effective head at any point.

$\{F(P)\}$ indicates that nodal force vector is dependent on flow pressure.

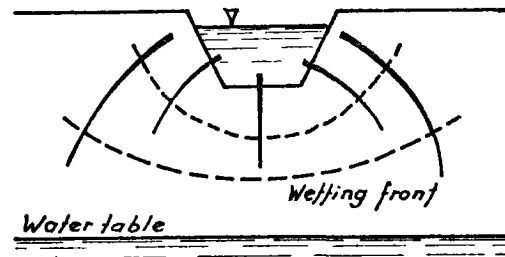
Then these two equations are coupled implicitly by $\{P\}$ and $\{\delta\}$.

UNSATURATED FLOW

Freesurf II cannot treat the problem of the transient flow through a dam when the reservoir level is lowered : this is due to the fact that the clay is draining very slowly and induces an unsaturated zone.



The unsaturated zone must also be taken into account if we consider the displacement of the wetting front during the infiltration process from a ditch into the ground.



As pollutants may migrate above the free surface as well as below, the presence of an unsaturated zone cannot be neglected in some pollution problems.

The moisture in soils is characterized by the following parameters :

i-the water content $\theta = \frac{V_w}{V_m}$, where V_w is the volume of water and

V_m the volume of the porous medium.

The maximum value of θ is the porosity of the medium

ii-the water saturation $S_w = \frac{V_w}{V_p}$, where V_p is the volume of the

pores ; $0 < S_w < 1$.

iii-the pressure head ψ , related to the piezometric head h and to the elevation z according to the formula :

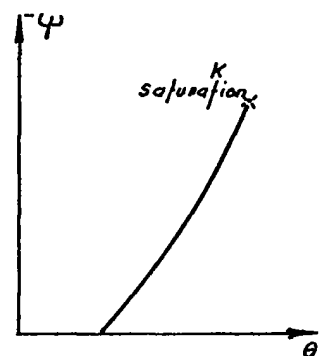
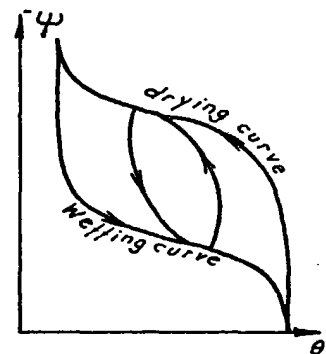
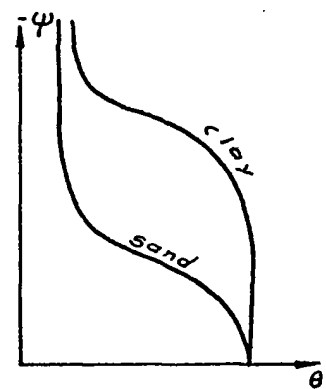
$$h = \psi + z$$

ψ , which is sometimes called suction or tension, is positive below the water table and negative above.

In the unsaturated zone, ψ is a function of θ whose shape depends on the porous medium.

In a given porous medium however we must take into account the hysteresis between ψ and θ : the actual curve ψ versus θ is comprised between a drying curve and a wetting curve according to the history of the flow.

The permeability K inside the unsaturated zone of an aquifer depends on the water content θ but the relationship between K and θ is extremely hard to measure.



One dimensional flow

When the soil is very dry the tension ψ is very high and the equations of flow in the unsaturated zone become extremely non linear.

According to the Buckingham-Darcy law and the definition of ψ the one dimensional continuity equation is :

$$\frac{\partial}{\partial z} \left[K \frac{\partial(\psi + z)}{\partial z} \right] = \frac{\partial \theta}{\partial t} \quad (1)$$

where z is positive upward.

ψ and θ being related, the usual approach in solving equation (1) is to express one of these two variables in terms of the other ; hence the two following possibilities :

i - express θ in terms of ψ : as ψ is continuous everywhere this approach fits for the solution of flow problems in both saturated and unsatu-

rated zones ; the equation however remains non linear.

ii - express ψ in terms of θ : as θ is constant within the saturated zone and may be discontinuous across two layers within the unsaturated zone, this approach enables us to solve only the flow in an unsaturated zone made of only one material ; the equation however is more linear than in the previous approach.

Let $D = K \frac{\partial \psi}{\partial \theta}$ be the diffusivity of the soil.

The 2nd approach leads to the equation :

$$\frac{\partial}{\partial z} \left(D \frac{\partial \theta}{\partial z} + K \right) = \frac{\partial \theta}{\partial t} \quad (2)$$

Let v be the velocity of water :

$$v = - K \frac{\partial h}{\partial z} = - K \frac{\partial (\psi + z)}{\partial z} = - K \frac{\partial \psi}{\partial z} - K = - D \frac{\partial \theta}{\partial z} - K$$

Let us note that in case of an horizontal flow along axis x the velocity would only have been :

$$v = - D \frac{\partial \theta}{\partial x}$$

The initial and boundary conditions of the problem are defined as follows :

$$\theta_{(z,0)} = \theta_0(z) \quad \text{on } R$$

$$\theta_{(z,t)} = \theta_{(z,t)} \quad \text{on } A_1$$

$$K \frac{\partial h}{\partial z} n_3 = (K + D \frac{\partial \theta}{\partial z}) n_3 = - V_{(z,t)} \quad \text{on } A_2$$

As K and D are functions of θ the problem is non linear and no variational principle is rigorously applicable.

As equation (2) involves θ in a linear fashion however the problem is quasi linear.

Let us apply Galerkin method ; we approximate θ by a linear combination θ^N of a set of N coordinate functions ξ_n :

$$\theta^N = \theta_n \xi_n$$

For any n, the function ξ_n is zero everywhere except along elements e_1 and e_2 where it varies linearly with z from zero at nodes n-1 and n+1 to 1 at node n.

Let us express that the projection of the residue of equation (2) along each coordinate function is zero :

$$\int_R \left[\frac{\partial}{\partial z} \left(D \frac{\partial \theta}{\partial z} + K \right) - \frac{\partial \theta}{\partial t} \right] \xi_n dR = 0 \quad (3)$$

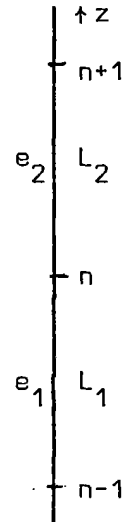
In order to solve this non linear problem by the finite element method and to avoid obtaining negative values for θ_n we must introduce the scalar :

$$\left(\frac{\partial \theta}{\partial t} \right)_n = \frac{\int_R \frac{\partial \theta}{\partial t} \xi_n dR}{\int_R \xi_n dR}$$

As θ is assumed to vary linearly along each element, let us make the same assumption for K and D :

$$K^e = K_n^e \xi_n^e$$

$$D^e = D_n^e \xi_n^e$$



Let us apply Green's first identity :

$$\int_R \frac{\partial}{\partial z} (D \frac{\partial \theta}{\partial z} + K) \xi_n dR + \int_R (D \frac{\partial \theta}{\partial z} + K) \frac{\partial \xi_n}{\partial z} dR = \int_{A_1+A_2} (D \frac{\partial \theta}{\partial z} + K) \xi_n \cdot n_3 dA$$

Equation (3) can then be rewritten as follows :

$$\sum_e \int_{R^e} \left[D_p^e \xi_p^e \frac{\partial \xi_m^e}{\partial z} \frac{\partial \xi_n^e}{\partial z} \theta_m + K_p^e \xi_p^e \frac{\partial \xi_n^e}{\partial z} + \frac{\partial \theta}{\partial t} \xi_n^e \right] dR = \sum_e \int_{A_1^e+A_2^e} (D_p^e \xi_p^e \frac{\partial \xi_m^e}{\partial z} \theta_m + K_p^e \xi_p^e) n_3 \xi_n^e dA$$

Hence :

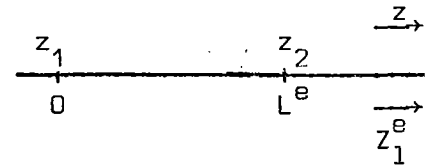
$$A_{nm} \theta_m + F_{nm} \frac{\partial \theta_m}{\partial t} = Q_n - B_n$$

Where :

$$A_{nm} = \sum_e \int_{R^e} D_p^e \xi_p^e \frac{\partial \xi_m^e}{\partial z} \frac{\partial \xi_n^e}{\partial z} dR$$

$$= \sum_e \frac{1}{2L^e} \frac{D_p^e}{p} (-1)^{\delta_{nm}+1} \quad 1_p D_p^e \text{ meaning } \sum_p D_p^e$$

The integration of ξ_p^e can be carried out in an easy way if we introduce the local coordinate Z_1^e ; L^e being the length of element e , the two coordinate functions which are non zero along the element are :



$$\xi_1^e = \frac{L^e - Z_1^e}{L^e} \quad \text{and} \quad \xi_2^e = \frac{Z_1^e}{L^e} \quad \text{where} \quad Z_1^e = z - z_1$$

$$F_{nm} = (\delta_{nm}) \sum_e \int_{R^e} \xi_n^e dR$$

$$= \delta_{nm} \sum_e \frac{L^e}{2}, \text{ the parentheses around } \delta_{nm} \text{ indicate that no}$$

summation is to be made on n .

The assumption made upon the integral of $\frac{\partial \theta}{\partial t}$ leads to a diagonal matrix F_{nm}

$$Q_n = \sum_e \int_{A_2^e} -V n_3 \xi_n^e dA + \sum_e \int_{A_1^e} \left(D_p^e \xi_p^e \frac{\partial \xi_m^e}{\partial z} \theta_m + K_p^e \xi_p^e \right) n_3 \xi_n^e dA$$

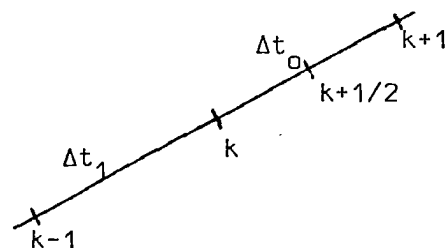
is the flux across the boundaries of the flow region ; it is positive when directed into the system.

$$B_n = \sum_e \int_R K_p^e \xi_p^e \frac{\partial \xi_n^e}{\partial z} dR$$

$$= \frac{1}{2} (K_{n-1} + K_n)^{e1} - \frac{1}{2} (K_n + K_{n+1})^{e2}$$

In order to solve this system of non linear equations we linearize by assuming that D and K remain constant within a given time step.

We use Rubin's method : we extrapolate values of θ from the previous time step through the present time step toward the next :



$$\frac{\theta^{k+1/2} - \theta^k}{\Delta t_0/2} = \frac{\theta^k - \theta^{k-1}}{\Delta t_1}$$

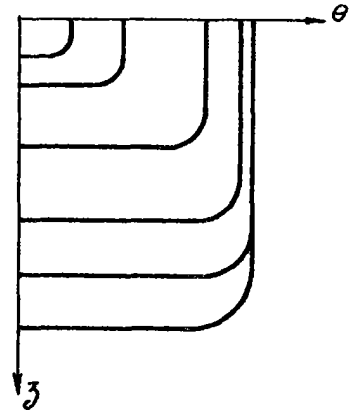
We use the extrapolated values $\theta^{k+1/2}$ in the calculation of D and K for time step Δt_0 . Hence the equation :

$$A_{nm}^{k+1/2} \frac{\theta_m^k + \theta_m^{k+1}}{2} + F_{nm}^{k+1/2} \frac{\theta_m^{k+1} - \theta_m^k}{\Delta t} = Q_n^{k+1/2} - B_n^{k+1/2}$$

The solution θ_m^{k+1} is then obtained without iteration.

The size of each time step is checked by calculating the material balance at the end of each time step.

This one dimensional scheme can be applied to the infiltration of rain into a very dry soil ; in the case of an infinite system, it comes to a translation of the wetting front.



Two dimensional flows

They are ψ based and cover the vertical plane flow, the vertical radial flow and the horizontal plane flow.

As very little is known about anisotropy in the unsaturated zone, we make the following assumption :

$K_{ij}(\theta) = K_{r(\theta)} K_{ij}^s$ where $0 < K_r < 1$ and K_{ij}^s is the permeability tensor in the saturated zone.

The pressure head ψ , which is continuous everywhere, is solution of the following equation :

$$\frac{\partial}{\partial x_i} \left(K_r K_{ij}^s \frac{\partial \psi}{\partial x_j} \right) + \frac{\partial}{\partial x_i} \left(K_r K_{i3}^s \right) = C \frac{\partial \psi}{\partial t} \quad (4)$$

Let us neglect hysteresis :

$$\frac{\partial \theta}{\partial t} = C \cdot \frac{\partial \psi}{\partial t} \quad \text{where } C = \frac{\partial \theta}{\partial \psi} \text{ is the specific moisture}$$

capacity, an highly non linear term.

Although there is no basic difference between left hand sides of equations (2) and (4), this ψ based method is no longer applicable to extremely dry media : this is due to term C in the right hand side of equation (4).

Rubin suggested a transformation which brings us back to the first type of equation.

In order to keep equation (4) however, we will restrict the study to non extremely dry soils.

Let us apply Galerkin's method :

$$\psi \approx \psi^N = \psi_n \xi_n$$

$$\int_R \left[\frac{\partial}{\partial x_i} \left(K_r K_{ij}^s \frac{\partial \psi}{\partial x_j} \right) + \frac{\partial}{\partial x_i} \left(K_r K_{i3}^s \right) - C \frac{\partial \psi}{\partial t} \right] \xi_n dR = 0$$

Green's first identity :

$$\begin{aligned} \int_R \left[\frac{\partial}{\partial x_i} \left(K_r K_{ij}^s \frac{\partial \psi}{\partial x_j} \right) + \frac{\partial}{\partial x_i} \left(K_r K_{i3}^s \right) \right] \xi_n dR + \int_R \left(K_r K_{ij}^s \frac{\partial \psi}{\partial x_j} + K_r K_{i3}^s \right) \frac{\partial \xi_n}{\partial x_i} dR \\ = \int_{A_1 + A_2} \left(K_r K_{ij}^s \frac{\partial \psi}{\partial x_j} + K_r K_{i3}^s \right) \xi_n n_i dA \end{aligned}$$

Let us assume :

$$\left(\frac{\partial \psi}{\partial t} \right)_n = \frac{\int_R C \frac{\partial \psi}{\partial t} \xi_n dR}{\int_R C \xi_n dR}$$

$$K_r^e = K_{rn}^e \xi_n^e$$

$$C^e = C_n^e \xi_n^e$$

Hence :

$$\sum_e \int_{R^e} \left[K_{rp}^e K_{ij}^s \xi_p^e \frac{\partial \xi_m^e}{\partial x_j} \frac{\partial \xi_n^e}{\partial x_i} \psi_m + K_{rp}^e K_{i3}^s \xi_p^e \frac{\partial \xi_n^e}{\partial x_i} + C_p^e \xi_p^e \frac{\partial \psi}{\partial t} \xi_n^e \right] dR$$

$$= \sum_e \int_{A_1^e + A_2^e} \left(K_{rp}^e K_{ij}^s \xi_p^e \frac{\partial \xi_m^e}{\partial x_j} \psi_m + K_{rp}^e K_{i3}^s \xi_p^e \right) n_i \xi_n^e dA$$

i.e. :

$$A_{nm} \psi_m + F_{nm} \frac{\partial \psi_m}{\partial t} = Q_n - B_n$$

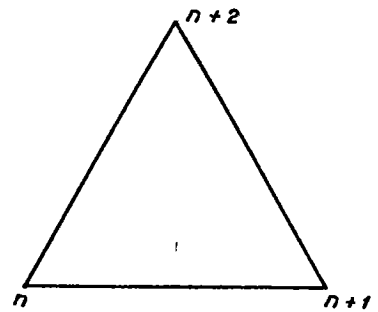
where :

$$A_{nm} = \sum_e K_{rp}^e K_{ij}^s \int_{R^e} \xi_p^e \frac{\partial \xi_m^e}{\partial x_j} \frac{\partial \xi_n^e}{\partial x_i} dR = \sum_e \frac{\alpha}{4\Delta} \bar{K}_r \left[K_{11}^s b_n b_m + K_{13}^s (b_n c_m + b_m c_n) + K_{33}^s c_n c_m \right]$$

K_{r1}, K_{r2}, K_{r3} being the values of K_r at nodes $n, n+1$ and $n+2$ of triangle e :

$$\bar{K}_r = \frac{1}{3} (K_{r1} + K_{r2} + K_{r3})$$

$$\alpha = \begin{cases} 1 & \text{for a plane flow} \\ 2\pi r & \text{for a radial flow} \end{cases}$$



$$F_{nm} = (\delta_{nm}) \sum_e \int_{R^e} C_p^e \xi_p^e \xi_n^e dR$$

$$= \delta_{nm} \sum_e \frac{\alpha \Delta}{12} (2c_n + c_{n+1} + c_{n+2})$$

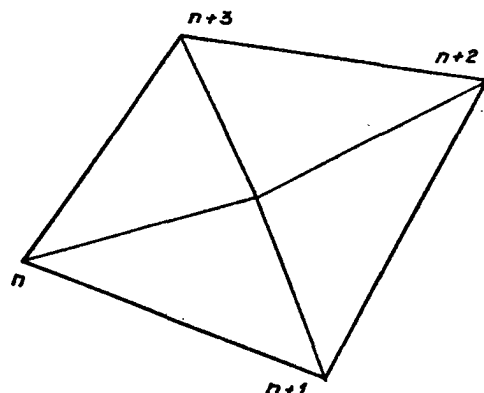
$$Q_n = \sum_e \int_{A_1^e + A_2^e} \left(K_{ij} \frac{\partial \psi}{\partial x_j} + K_{i3} \right) n_i \xi_n^e dA$$

$$B_n = \sum_e K_{rp}^e K_{i3}^s \int_e \xi_p^e \frac{\partial \xi_n^e}{\partial x_i} dR$$

$$= \sum_e \frac{\alpha}{2} \bar{K}_r (K_{13}^s b_n + K_{33}^s c_n) \quad (B_n = 0 \text{ for an horizontal plane flow problem}).$$

plane flow problem).

For a quadrilateral element the values of c and K at the middle point are reported on the four summits and set equal to zero ; this enables us to eliminate the middle points.



By analogy with the general case :

$$F_{nm} = (\delta_{nm}) \sum_e \frac{\alpha \Omega}{20} (2c_n + c_{n+1} + c_{n+2} + c_{n+3})$$

ψ being assumed to vary linearly with time, we use Rubin's method again :

$$\left(A_{nm}^{k+1/2} + \frac{2}{\Delta t} F_{nm}^{k+1/2} \right) \cdot \psi_m^{k+1} = 2 Q_n^{k+1} - 2 B_n^{k+1/2} - \left(A_{nm}^{k+1/2} - \frac{2}{\Delta t} F_{nm}^{k+1/2} \right) \cdot \psi_m^k \quad (5)$$

A S_s term could be easily incorporated into this equation.

As equation (5) is not strictly linear we have 3 possibilities :

i - iterate without checking the material balance. By extrapolation from the value of ψ at time step $k-1$ through its value at time step k we calculate $\psi^{k+1/2}$; we then evaluate $C^{k+1/2}$ and $K_r^{k+1/2}$, then matrices $A^{k+1/2}$, $F^{k+1/2}$ and $B^{k+1/2}$ and we finally solve equation (5) for ψ^{k+1} .

We correct the evaluation of matrices A , F and B using $\frac{\theta^k + \theta^{k+1}}{2}$ and solve equation (5) again.

We iterate until the difference between two successive evaluations of θ^{k+1} is less than a prescribed test value.

This scheme insures an extremely rapid convergence.

ii - make only one iteration and then check the material balance :
if the discrepancy is larger than a prescribed test value we iterate as in i
and no more check the material balance.

iii - check material balance after each time step : if the discrepancy
is too large, dump results on a tape

Calculation of the material balance

Let V_e be the change in storage in element e :

$$V_e = \int_{R^e} \int_t^{t+\Delta t} \frac{\partial \theta}{\partial t} dt dR$$

If we assume that θ varies linearly with time :

$$V_e = \alpha \left\{ \begin{array}{c} \Delta \\ \square \end{array} \right\} \left(\frac{1}{\theta^{k+1}} - \frac{1}{\theta^k} \right)$$

The material balance is then :

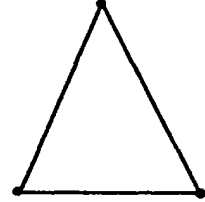
$$\sum_e V_e = \Delta t \cdot \sum_n Q_n$$

We compute the difference between the two terms and compare it to
zero.

VARIOUS INTERPOLATION SCHEMES

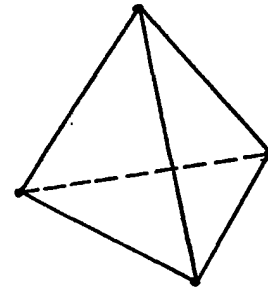
Simplex element :

In the two dimensional case it can be a triangle with 3 nodes ; the line joining any two points on the boundary belongs to the element : the triangle is a convex element.



In the three dimensional case it can be a tetraedral element with 4 nodes.

In general, the number N^e of nodes of a simplex element is related to the dimension K of the space according to the formula :



$$N^e = K + 1$$

The coordinate functions associated with a simplex element are defined by the relations :

$$\xi_n^e(x_i^m) = \delta_{nm}$$

$$\sum_{n=1}^{N^e} \xi_n^e(x_i) = 1 \quad \forall x_i \in R^e$$

ξ_n^e can be expressed by a polynomial of degree 1 i.e. by a linear function of coordinates x_i :

$$\xi_n^e(x_i) = a_0^n + a_i^n x_i \quad i = 1 \dots k$$

The constant coefficients a are determined by identification at the nodes :

$$a_0^n + a_i^n x_i^n = \delta_{nm}$$

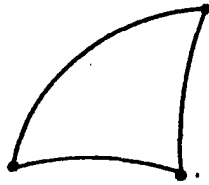
In the two dimensional case for instance :

$$\xi_n^e(x_i) = a_0^n + a_1^n x_1 + a_2^n x_2$$

the three unknowns a_0^n , a_1^n and a_2^n are the solutions of the three linear equations :

$$\xi_n^e \left(\begin{matrix} x \\ i \end{matrix} \right) = \delta_{nm}$$

We can define simplex elements in curvilinear coordinates, on a sphere for instance :

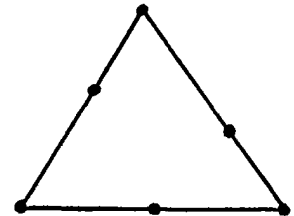


Complex element :

For such an element the relationship between the number of the nodes and the dimension of the space is the following :

$$N^e > K + 1$$

For instance, in a two dimensional space, a triangle with 6 nodes is a complex element.



Although this assumption is not necessary, we will restrict ourselves to polynomial expressions. Let m be the degree of such a polynomial. For the above triangular complex element $m = 2$:

$$\xi_n^e(x_i) = a_0^n + a_1^n x_1 + a_2^n x_2 + a_3^n (x_1)^2 + a_4^n (x_1 x_2) + a_5^n (x_2)^2$$

We will determine the coefficients by using the Lagrange interpolation.

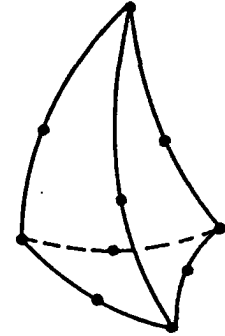
To the 6 unknowns correspond 6 linear equations :

$$\xi_n^e \left(x_i^m \right) = \delta_{nm}$$

The unicity of the solution is thus insured. Curvilinear coordinates may also be used.

The continuity of the unknown function is insured accross the boundaries of any element.

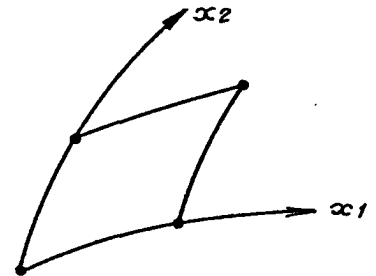
ex. : a parabolic expression along the boundary of a triangle is valid in each adjacent triangle.



Multiplex element :

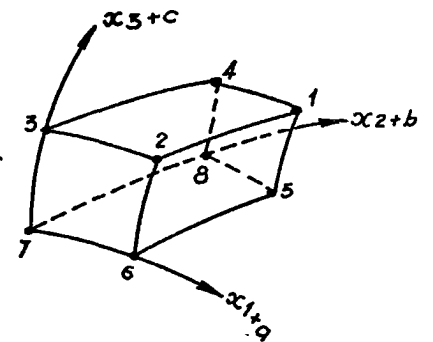
The boundaries of such an element are parallel to the coordinate axes.

In a two dimensional space we use a bilinear interpolation : the coordinate function is assumed to vary linearly along the boundaries of the element but not necessarily inside.



$$\xi_n^e (x_i) = a_0^n + a_1^n x_1 + a_2^n x_2 + a_3^n x_1 x_2$$

In a three dimensional space a trilinear interpolation leads to the following coordinate functions :



$$\xi_n^e (x_i) = a_0^n + a_1^n x_1 + a_2^n x_2 + a_3^n x_3 + a_4^n x_1 x_2 + a_5^n x_1 x_3 + a_6^n x_2 x_3 + a_7^n x_1 x_2 x_3$$

Let $x_1 = \pm a$ $x_2 = \pm b$ $x_3 = \pm c$ be the equations of the boundaries ; we then define adimensional local coordinates as follows :

$$\alpha = \frac{x_1}{a} , \quad \beta = \frac{x_2}{b} , \quad \gamma = \frac{x_3}{c}$$

The interpolation leads to the following functions :

$$\xi_1^e = \frac{1}{8} (1 + \alpha) (1 + \beta) (1 + \gamma)$$

$$\xi_2^e = \frac{1}{8} (1 + \alpha) (1 - \beta) (1 + \gamma)$$

$$\xi_3^e = \frac{1}{8} (1 - \alpha) (1 - \beta) (1 + \gamma)$$

$$\xi_4^e = \frac{1}{8} (1 - \alpha) (1 + \beta) (1 + \gamma)$$

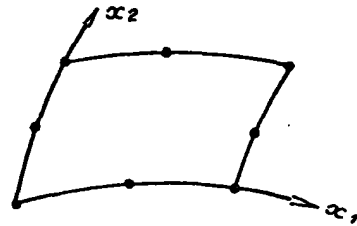
$$\xi_5^e = \frac{1}{8} (1 + \alpha) (1 + \beta) (1 - \gamma)$$

$$\xi_6^e = \frac{1}{8} (1 + \alpha) (1 - \beta) (1 - \gamma)$$

$$\xi_7^e = \frac{1}{8} (1 - \alpha) (1 - \beta) (1 - \gamma)$$

$$\xi_8^e = \frac{1}{8} (1 - \alpha) (1 + \beta) (1 - \gamma)$$

In a two dimensional space a biquadratic interpolation can be carried out with 8 nodes.



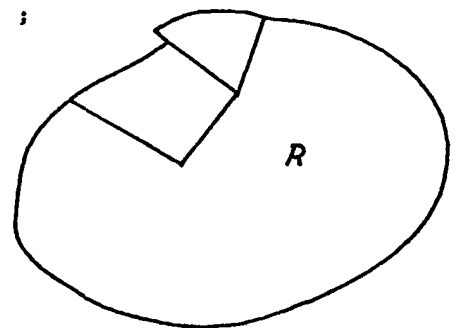
Isoparametric elements :

They were introduced in 1968 by Ergatoudis, Irons and Zienkiewicz.

Definition :

The elements are chosen in a region R ;
in each of these elements the local coordinates
are parallel to the boundaries of the element.

We can make a transformation from
Cartesian coordinates x_i into local coordinates
 α_i and vice versa :



$$\alpha_i = \alpha_i(x_i) \quad x_i = x_i(\alpha_i)$$

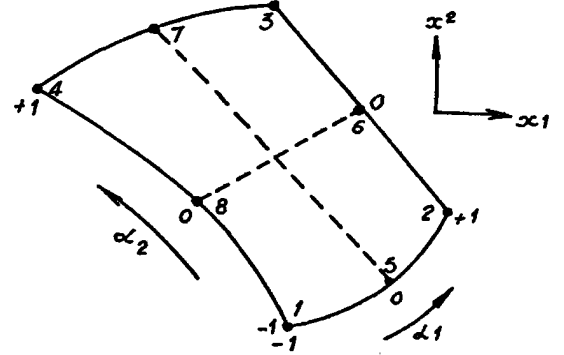
Biquadratic interpolation :

Let us number 8 nodes inside the element ; we assume the relationship :

$$x_i = a_0^i + a_1^i \alpha_1 + a_2^i \alpha_2 + a_3^i (\alpha_1)^2 + a_4^i (\alpha_1 \alpha_2) + a_5^i (\alpha_2)^2 + a_6^i (\alpha_1)^2 \alpha_2 + a_7^i \alpha_1 (\alpha_2)^2$$

Substituting the coordinates of the 8 nodes into the above expression leads to 8 linear equations whose solutions are the 8 unknowns a.

It is also possible to express α in terms of x .



The interpolation functions are usually obtained by guessing

$$\xi_n^e(\alpha_i) = \frac{1}{4} \left[(1 + \alpha_1 \alpha_1^n)(1 + \alpha_2 \alpha_2^n) - (1 - (\alpha_1)^2)(1 + \alpha_2 \alpha_2^n) - (1 + \alpha_1 \alpha_1^n)(1 - (\alpha_2)^2) \right] \quad n=1,2,3,4$$

$$\xi_n^e(\alpha_i) = \frac{1}{2} (1 - (\alpha_1)^2) (1 + \alpha_2 \alpha_2^n) \quad n = 5, 7$$

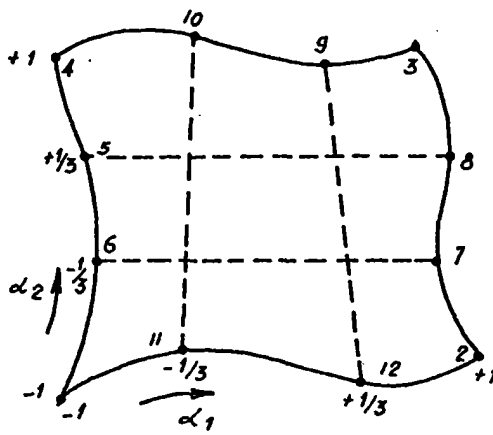
$$\xi_n^e(\alpha_i) = \frac{1}{2} (1 - (\alpha_2)^2) (1 + \alpha_1 \alpha_1^n) \quad n = 6, 8$$

We can check that $\xi_n^e(\alpha_i^m) = \delta_{nm}$

Bicubic interpolation :

$N^e = 12$; the relation between x_i and α_i is obtained by analogy with the quadratic interpolation.

$$x_i = a_0^i + a_1^i \alpha_1 + a_2^i \alpha_2 + a_3^i (\alpha_1)^2 + a_4^i (\alpha_1 \alpha_2) + a_5^i (\alpha_2)^2 + a_6^i (\alpha_1)^2 \alpha_2 + a_7^i \alpha_1 (\alpha_2)^2 + a_8^i (\alpha_1)^3 + a_9^i \alpha_1 (\alpha_2)^3 + a_{10}^i (\alpha_1)^3 \alpha_2 + a_{11}^i (\alpha_2)^3$$



The coordinate functions then are :

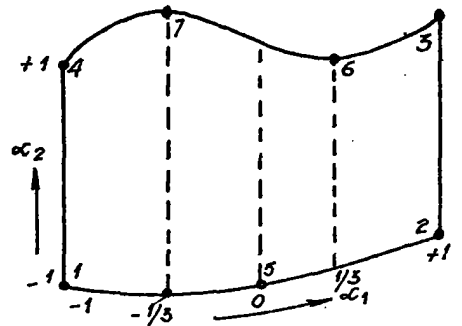
$$\xi_n^e(\alpha_1) = \frac{1}{32} (1 + \alpha_1 \cdot \alpha_1^n) (1 + \alpha_2 \cdot \alpha_2^n) \left\{ 9 \left[(\alpha_1)^2 + (\alpha_2)^2 \right] - 10 \right\} \quad n = 1, 2, 3, 4$$

$$\xi_n^e(\alpha_1) = \frac{9}{32} (1 + \alpha_1 \alpha_1^n) \left[1 - (\alpha_2)^2 \right] (1 + 9\alpha_2 \alpha_2^n) \quad n = 5, 6, 7, 8$$

$$\xi_n^e(\alpha_1) = \frac{9}{32} (1 + 9\alpha_1 \alpha_1^n) \left[1 - (\alpha_1)^2 \right] (1 + \alpha_2 \alpha_2^n) \quad n = 9, 10, 11, 12$$

Mixed interpolation :

It is possible to use different orders of interpolation along the boundaries of a given element.



order of the interpolation	$b_n(\alpha)$
linear	$\frac{1}{2}$
quadratic	$\alpha \alpha^n - \frac{1}{2}$
cubic	$\frac{1}{8} \left(9(\alpha)^2 - 5 \right)$

Let us take, for instance, the following example :

- linear interpolation at nodes $n = 1, 2, 3, 4$

$$\xi_n^e(\alpha_i) = (a_n) (b_n)$$

there is no summation here

where :

$$a_n = \frac{1}{4} (1 + \alpha_1 \alpha_1^n) (1 + \alpha_2 \alpha_2^n)$$

$$b_n = b_n(\alpha_1) + b_n(\alpha_2)$$

- quadratic interpolation at node $n = 5$

$$\xi_n^e(\alpha_i) = \frac{1}{2} \left[1 - (\alpha_1)^2 \right] \left[1 + \alpha_2 \alpha_2^n \right]$$

- cubic interpolation at nodes $n = 6, 7$

$$\xi_n^e(\alpha_i) = \frac{9}{32} \left[1 - (\alpha_1)^2 \right] \left[1 + 9 \alpha_1 \alpha_1^n \right] \left[1 + \alpha_2 \alpha_2^n \right]$$

Integration over an element :

As the local coordinates vary only from -1 to +1, the integration of the coordinate functions is simplified :

$$\int_{R^e} \xi_n^e(\alpha_i) d\alpha_1 d\alpha_2 = \int_{-1}^1 d\alpha_1 \int_{-1}^1 \xi_n^e(\alpha_i) d\alpha_2$$

In order to integrate derivatives of ξ_n^e with respect to cartesian coordinates we must introduce the Jacobian matrix J

$$J = \begin{bmatrix} \frac{\partial x_1}{\partial \alpha_1} & \frac{\partial x_2}{\partial \alpha_1} \\ \frac{\partial x_1}{\partial \alpha_2} & \frac{\partial x_2}{\partial \alpha_2} \end{bmatrix}$$

$$\begin{bmatrix} \frac{\partial \xi_n^e}{\partial x_1} \\ \frac{\partial \xi_n^e}{\partial x_2} \end{bmatrix} = J^{-1} \begin{bmatrix} \frac{\partial \xi_n^e}{\partial \alpha_1} \\ \frac{\partial \xi_n^e}{\partial \alpha_2} \end{bmatrix}$$

Numerical integration is necessary in order to evaluate the integral.

An easy way to calculate the derivatives $\frac{\partial x_i}{\partial \alpha_j}$ is to express x_i in terms of a linear combination of x_i^n :

$$x_i = \xi_n^e(\alpha_i) \cdot x_i^n$$

Such an expression is correct because ξ_n^e is an interpolation function and x_i is supposed to be a polynomial of the same order as the unknown along the boundaries.

Hermite interpolation :

Smooth Hermite interpolation :

In the one dimensional case, the unknown h is approximated by a linear combination of two sets of N coordinate functions ξ_n and ζ_n :

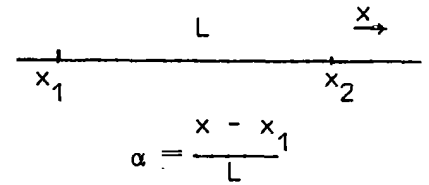
$$h = h^N = h_n \xi_n + h'_n \zeta_n \quad \text{where} \quad h'_n = \left(\frac{\partial h}{\partial x} \right)$$

The coordinate functions are defined according to the following relations where prime means derivative with respect to x_i :

$$\begin{aligned} \xi_n(x_i^m) &= \delta_{nm} & \zeta_n(x_i^m) &= 0 \\ \xi'_n(x_i^m) &= 0 & \zeta'_n(x_i^m) &= \delta_{nm} \end{aligned}$$

This interpolation makes the derivative h' to be continuous at the nodes (\rightarrow smooth interpolation).

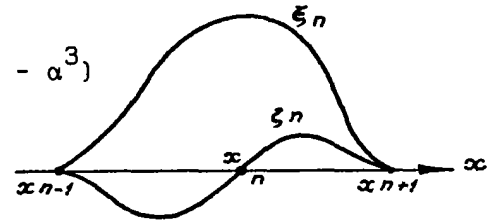
α being a local coordinate associated with a given element, a smooth cubic interpolation leads to the following coordinate functions :



$$\xi_1^e = 1 - 3\alpha^2 + 2\alpha^3 \quad \zeta_1^e = L(\alpha - 2\alpha^2 + \alpha^3)$$

$$\xi_2^e = 3\alpha^2 - 2\alpha^3 \quad \zeta_2^e = -L(\alpha^2 - \alpha^3)$$

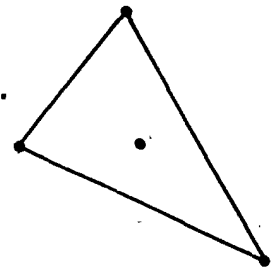
where L is the length of the element.



The shape of the two coordinate functions associated with a given node n is shown on the above figure.

In general, using a polynomial of degree $n + 2$ insures that in the one dimensional case derivatives of h until the n^{th} order are continuous.

In the two dimensional case, when elements are triangles, the centroid of each element is a node. A m^{th} order Hermite polynomial corresponds to polynomials of degree $2m - 1$.



Let $\xi_{n,jk}^e$ be the coordinate function associated with node n and corresponding to the derivative of h of order j with respect to x_1 and of order k with respect to x_2 . By using only one greek alphabetic character this notation generalizes the notation (using ξ and ζ) defined in the one dimensional case.

Unknown h is then approximated as a linear combination of a set of N coordinate functions $\xi_{n,jk}^e$:

$$h \approx h^N = \sum_{n,jk} h_{n,jk} \xi_{n,jk}^e \quad \text{where} \quad h_{n,jk}(t) = \frac{\partial^{j+k} h}{\partial x_1^j \partial x_2^k} (x_i^n, t)$$

The corner nodes

$m - 1$ is the maximum order of the derivatives of h that we want to be continuous at each corner node :

$$0 \leq j, k \leq m - 1.$$

The corresponding coordinate functions satisfy the following relation :

$$\left(\frac{\partial^{\bar{j}+\bar{k}} \xi_{n,jk}}{\partial x_1^{\bar{j}} \partial x_2^{\bar{k}}} \right) \left(x_i^{\bar{n}} \right) = \delta_{n\bar{n}} \delta_{j\bar{j}} \delta_{k\bar{k}}$$

The number of coordinate functions associated with a corner node is $\frac{m(m+1)}{2}$.

Examples :

If the function itself only is to be set continuous, $m = 1$ and we define only one coordinate function $\xi_{n,00}$:

$$\xi_{n,00} \left(x_i^{\bar{n}} \right) = \delta_{n\bar{n}}$$

If we want the function together with its two first order derivatives to be continuous, $m = 2$ and we define the following coordinate functions.

$\xi_{n,00}$ associated with the function itself

$$\left(\frac{\partial^{\bar{j}+\bar{k}} \xi_{n,00}}{\partial x_1^{\bar{j}} \partial x_2^{\bar{k}}} \right) \left(x_i^{\bar{n}} \right) = \delta_{n\bar{n}} \delta_{0\bar{j}} \delta_{0\bar{k}}$$

$\xi_{n,10}$ associated with $\frac{\partial h}{\partial x_1}$

$$\left(\frac{\partial^{\bar{j}+\bar{k}} \xi_{n,10}}{\partial x_1^{\bar{j}} \partial x_2^{\bar{k}}} \right) \left(x_i^{\bar{n}} \right) = \delta_{n\bar{n}} \delta_{1\bar{j}} \delta_{0\bar{k}}$$

$\xi_{n,01}$ associated with $\frac{\partial h}{\partial x_2}$

$$\left(\frac{\partial^{\bar{j}+\bar{k}} \xi_{n,01}}{\partial x_1^{\bar{j}} \partial x_2^{\bar{k}}} \right) \left(x_i^{\bar{n}} \right) = \delta_{n\bar{n}} \delta_{a\bar{j}} \delta_{1\bar{k}}$$

so that h might be approximated by h^N as follows :

$$h \approx h^N = h_n \xi_{n,00} + \left(\frac{\partial h}{\partial x_1} \right)_n \xi_{n,10} + \left(\frac{\partial h}{\partial x_2} \right)_n \xi_{n,01}$$

The centroid

$m - 2$ is the maximum order of the derivatives of h we want to be continuous at each centroid :

$$0 \leq j, k \leq m - 2$$

The number of coordinate functions associated with such a node is then $\frac{m(m-1)}{2}$.

These coordinate functions have the same properties as those associated with corner nodes.

In general :

The method leads to a N -dimensional subspace of the Hermit space.

For triangular elements, if N_c and N_o are the numbers of the corner nodes and of the centroids respectively :

$$N = N_c \frac{m(m+1)}{2} + N_o \frac{m(m-1)}{2}$$

The function h is then approximated as follows :

$$h \approx h^N = \left(\sum_{n=1}^{N_c} \sum_{j=0}^{m-1} \sum_{k=0}^{m-1} + \sum_{n=1}^{N_o} \sum_{j=0}^{m-2} \sum_{k=0}^{m-2} \right) h_{n,jk}(t) \xi_{n,jk}(x_i)$$

Non smooth Hermit interpolation :

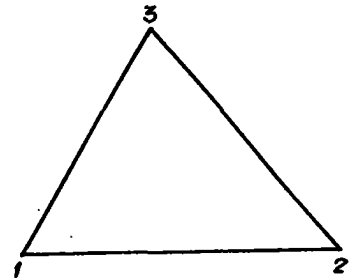
Let us suppose that, for a given element e , a smooth Hermit interpolation has been defined ; this interpolation is extended by a set of coordinate functions \varnothing_{ei} which are zero along the boundaries of the element.

This scheme does not change anything in the Lagrange interpolation :

$$\xi_{n(x_i^m)}^* = \xi_{n(x_i^m)} + \zeta_{(x_i^m)} = \delta_{nm} \quad \text{as } \zeta_{(x_i^m)} = 0 .$$

Let us consider a cubic interpolation for a triangle :

$$\varnothing_{e1} = \xi_1^e \quad \xi_2^e \quad \xi_3^e$$



The unknown function h is interpolated as follows :

$$h = \xi_1 h_1 + \xi_2 h_2 + \xi_3 h_3 + \varnothing_{e1} a_1 , \text{ which is still a Lagrange scheme.}$$

This non smooth interpolation is done in each triangle separately and not necessarily in all of them.

This scheme could be applied in an unsaturated flow problem when one wants a better approximation of the unknown inside the elements close to the wetting front.

A quintic interpolation for a triangle leads to the following coordinate functions:

$$\begin{aligned} \varnothing_{e1} &= \left(\xi_1^e\right)^3 \quad \xi_2^e \quad \xi_3^e , & \varnothing_{e2} &= \left(\xi_1^e\right)^2 \quad \left(\xi_2^e\right)^2 \quad \xi_3^e , & \varnothing_{e3} &= \xi_1^e \quad \left(\xi_2^e\right)^3 \quad \xi_3^e \\ \varnothing_{e4} &= \xi_1^e \quad \left(\xi_2^e\right)^2 \quad \left(\xi_3^e\right)^2 , & \varnothing_{e5} &= \xi_1^e \quad \xi_2^e \quad \left(\xi_3^e\right)^3 , & \varnothing_{e6} &= \left(\xi_1^e\right)^2 \quad \xi_2^e \quad \left(\xi_3^e\right)^2 . \end{aligned}$$

For steady state flow or unsteady state using vector D_n instead of matrix D_{nm} the interpolation leads to two sets of independent equations:

$$A_{nm} h_m = Q_n \quad (1)$$

$$\bar{A}_{nm} a_m = \bar{Q}_n \quad (2)$$

We first solve (1) for any node and then solve (2) for appropriated elements.

This interpolation scheme has been used by Price, Cavendish and Varga for one dimensional dispersion.

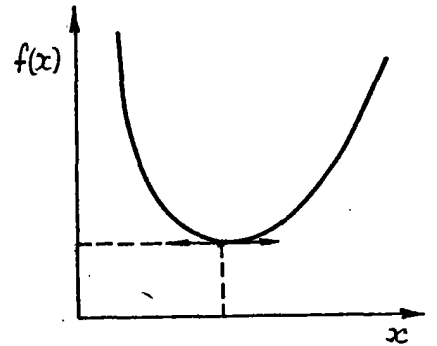
APPENDICE 1 - MEANING OF λ IN THE EXPRESSION OF Ω

For the free surface, we calculate

$$\delta\Omega(h) = \left. \frac{d}{d\lambda} (\Omega(h + \lambda\tilde{h})) \right|_{\lambda=0} \quad *$$

In calculus of variations, we have a relation between a functional Ω and a function R .

Let us consider in 2 dimensions a function $f(x)$.



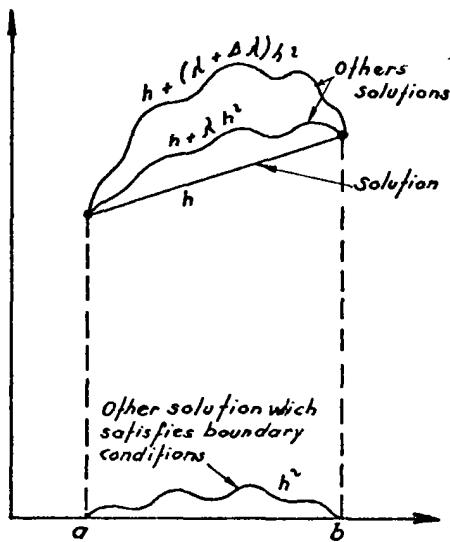
An extremum is obtained when :

$$\frac{df}{dx} = 0$$

with

$$\frac{df}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

It appears the same relationship between the functional Ω and the function h and between the function f and the point x .



Let us suppose that we have the solution h of the variational principle.

If \tilde{h} is an arbitrary function which satisfies boundary conditions, we can obtain all the possible solutions.

Let us evaluate

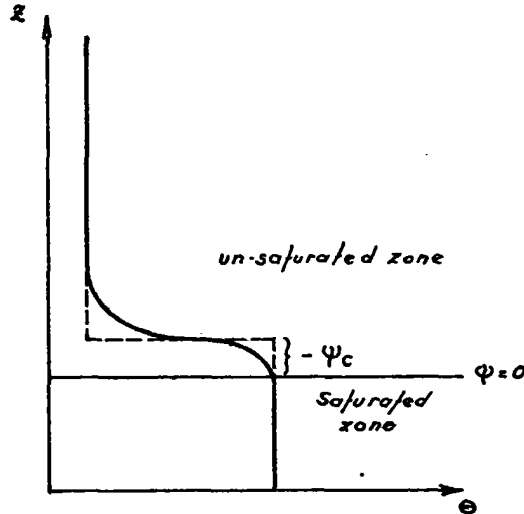
$$\lim_{\Delta\lambda \rightarrow 0} \frac{\Omega(h + (\lambda + \Delta\lambda)\tilde{h}) - \Omega(h + \lambda\tilde{h})}{\Delta\lambda}$$

This limit is called the first variation.

* book by FDMIN about variational principle.

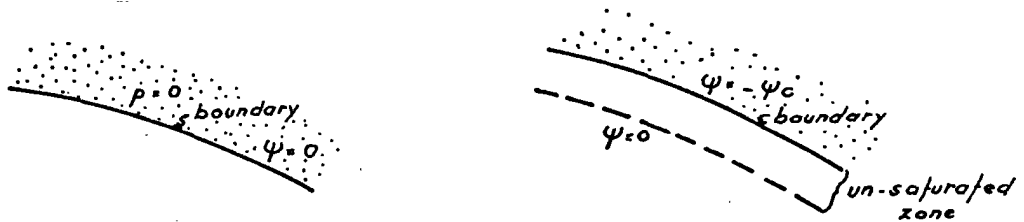
APPENDICE 2 - UNSATURATED ZONE

In some studies, we may be obliged to take into account the unsaturated zone. For the unsaturated zone, we have the relation between the percentage of water in the soil (θ) and the distance above the free surface, as indicated on the figure.



So, we assume during the iterations that the potential at the free surface boundary may be $\psi = -\psi_c$.

If there is no un-saturated zone, the value of ψ on the boundary is $\psi = 0$.



a) without un-saturated zone

b) with saturated zone

free surface positions

APPENDICE 3 - METHODS FOR SOLVING LINEAR EQUATIONS

- 1) In direct methods, it is possible to obtain an algorithm for getting a solution, but in such cases, we must consider the problem of roundoff error.
- 2) In iterative methods, it exists explicit equations for head at each node.

2.1.) Point Jacobi method

$$h_i^{m+1} = - \sum_{\substack{j=1 \\ j \neq i}}^N \left(\frac{a_{ij}}{a_{ii}} \right) h_j^m + \frac{b_i}{a_{ii}} \quad i= 1,2,\dots$$

The number m indicate the number of the iteration.

2.2.) Point Gauss-Seidel method

$$h_i^{m+1} = - \sum_{j=1}^{i-1} \left(\frac{a_{ij}}{a_{ii}} \right) h_j^{m+1} - \sum_{i+1}^N \left(\frac{a_{ij}}{a_{ii}} \right) h_j^m + \frac{b_i}{a_{ii}}$$

2.3.) Point successive over relaxation method

$$\begin{aligned} h_i^{m+1} &= h_i^m + w (h_i^{m+1} - h_i^m) \\ &= (1-w) h_i^m + w h_i^{m+1} \end{aligned}$$

- if $0 < w < 1$ we have an under-relaxation method
 $w = 1$ " " the Gauss-Seidel relaxation
 $1 < w < 2$ " " an over relaxation method.