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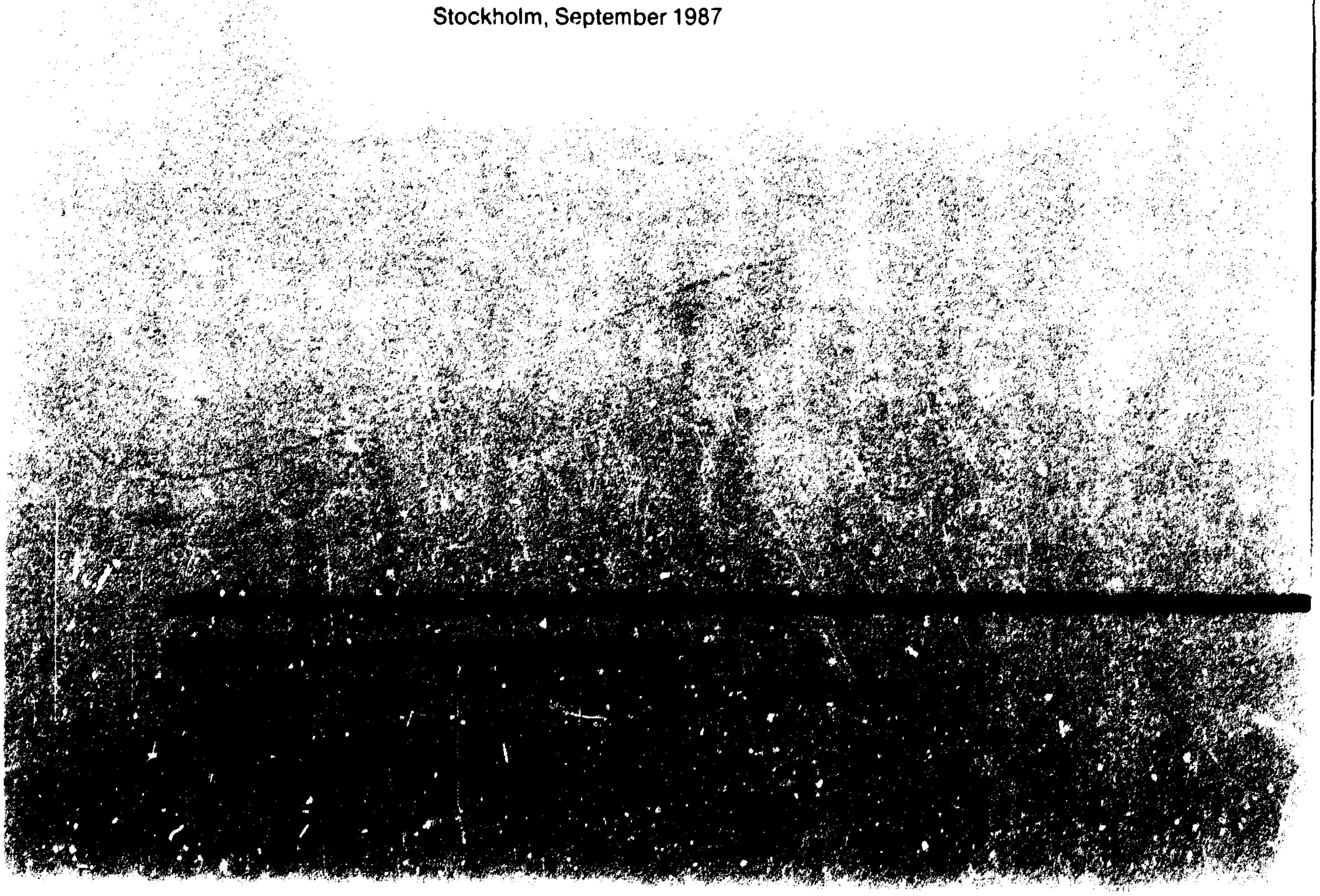
Calculation of gas migration in fractured rock – a continuum approach

Carol Braester
Israel Institute of Technology
Haifa, Israel

Roger Thunvik
Royal Institute of Technology
Stockholm, Sweden

Stockholm, September 1987



CALCULATION OF GAS MIGRATION IN FRACTURED ROCK - A CONTINUUM APPROACH

Carol Braester
Israel Institute of Technology
Haifa, Israel

Roger Thunvik
Royal Institute of Technology
Stockholm, Sweden

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Carol Braester
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ABSTRACT

A study of gas migration from low level radioactive repositories in which the fractured rock mass was conceptualized as a continuum, was carried out by the aid of a computer program based on a finite difference numerical method of solution to the equations of flow. The displacement is considered to be governed by the equations of simultaneous two-phase flow, gas and water. Without having the possibility of practical determination of the parameters of the continuum equivalent such as capillary pressure and relative permeabilities of the fractured rock, these functions were assumed. The calculations are intended to correspond to the prevailing in the Forsmark low level repository area where radioactive waste repository caverns are planned to be located at a depth of about 50 metres below the sea level. Chemical reactions in the stored waste will result in gas (hydrogen) production in a saturated water environment. Under such conditions the gas will displace the water from the rock and migrate towards the surface and finally be released through the sea bottom. Calculations were worked out for a constant gas flow rate equivalent to a gas production of 20000 normal cubic metres per year. The investigated flow domain was a vertical cross-section passing through the repository. The results show that in the empty cavern the gas formed in the cavern moves almost instantaneously upward and accumulates below the roof of the cavern. The gas penetrates the rock and displaces the water after a gas cushion of 0.4 m, corresponding to the assumed entry capillary pressure value, is formed below the roof of the cavern. In the cavern, the gas-water interface is horizontal. The gas advance is faster in the centre of the repository than at the edges. The displacement is limited to the near region to the repository. The breakthrough time at the sea bottom is about 0.6 days. The results are different from thos obtained in the previous studies in which the rock was conceptualized as a discrete system of fractures in which the flow process is dominated by the largest fractures and as a consequence the breakthrough time is smaller.

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NOMENCLATURE

symbol	description	dimension
c_w	compressibility of the fluid	$M^{-1}Lt^{2}$
c_r	compressibility of the rock matrix	$M^{-1}Lt^{2}$
g	acceleration of gravity	Lt^{-2}
k	permeability	L^{2}
M	molecular weight of the gas	$M\ mole^{-1}$
p	pressure	$ML^{-1}t^{-2}$
p_c	capillary pressure	$ML^{-1}t^{-2}$
Q	mass rate of flow	$ML^{-3}t^{-1}$
R	gas constant	$ML^{2}t^{-2}T^{-1}mole^{-1}$
t	time	t
S	saturation	-
T	temperature	T
u	volumetric rate of flow per unit area	Lt^{-1}
Z	correction factor for real gases	$^{-1}$-

Greek	description	dimension
ρ	density	ML^{-3}
μ	dynamic viscosity	$ML^{-1}t^{-1}$
ϕ	porosity	-

subscripts	
w	water
g	gas
r	rock

1. INTRODUCTION

In the previous studies on gas migration from low level radioactive repositories (SKBF-KBS: 83-21, SFR-Progress Report 86-04), the rock mass was conceptualized as a discontinuous system of fracture planes intersecting the rock cavern. The discrete approach was considered to represent better the actual flow phenomena associated with gas-water displacement in a fractured rock mass than the continuum approach. However parallel studies using the continuum approach were carried out by Intera (1986).

The result presented by Intera exhibited some unexpected flow phenomena requiring further investigation before being accepted. This implies in particular the unrealistic results obtained for the saturation distribution (Intera 1986, Fig. 4.6) which showed a faster displacement of the gas at the edges of the repository than in the centre. It is obvious that with an unrealistic saturation distributions all the other results e.g., the breakthrough time of the gas at the sea bottom are unreliable.

It was therefore decided to perform a comparative study using same data as those used by Intera in order to study if the flow phenomena reported could have any physical foundation or must have been the result of conceptual mistakes in the modelling. The present study demonstrates that the flow phenomena stated by Intera have no foundation whatsoever. Moreover, it was possible to reconstruct the mistake made in the modelling which caused the spurious results presented.

The study was carried by using Nolen's two-phase V.I.P. - Vectorized Implicit Program. The results of the present calculations are in total agreement with the actual physical behaviour of the flow process but not in agreement with the results obtained by Intera.

The gas (hydrogen) generated in the cavern is due to chemical reactions in the stored waste. The gas will be produced in a saturated water environment and due to the difference in density with respect to the water, the gas will migrate upward and finally escape through the sea bottom. The calculations presented here are intended to correspond to the prevailing in the Forsmark area.

In the discrete approach with a fracture width distribution the flow is dominated by the fractures of high permeability. In the present study with the continuum approach the rock is considered homogeneous so that under similar conditions the displacement is identical in any cross-section through an ideal cavern of infinite extent. The cavern is considered to have a horizontal roof and is treated as an empty cavity.

Being theoretically of infinite permeability, the gas formed in some part of the cavern will spread almost instantaneously along the cavern. The length of the cavern is more than 10 times larger than its height and its width, so that practically, with except to the ends of the cavern, the rest of it will behave like one of an infinite extent. For these reason the flow pattern through a two-dimensional vertical cross section passing the repository may be considered to be representative for the flow pattern.

Gas-water displacement is a non-wetting - wetting fluid displacement, so that a pressure entry value or a threshold pressure should be reached to initiate the displacement. Such an overpressure in the gas phase is equivalent to the formation of a gas cushion of a certain thickness in the cavern. This threshold pressure is dictated by the capillary pressure, a function of fluid saturation and of the formation under the consideration, conceptualized as as a continuum.

The continuum approach also requires that relative permeabilities for gas and water functions of saturation be supplied. Since it is impossible to determine a capillary pressure curve or relative permeability curves for a fractured rock these functions have to be assumed.

In the continuum approach the rock properties values represent average values of an elementary rock volume. The present study is carried out using a finite difference method of solution which requires a discretization of the flow domain in a number of grid blocks. The discretization mesh considered by Intera, and also in this study, includes small sizes of the blocks, down to 0.1 by 0.1 m.

Such a discretization, including small sizes of the blocks in some regions, is necessary to obtain accurate numerical solutions. As the representative size of an elementary block of a fractured rock formation is at least of order of magnitude of meters and it should be obvious that transient solution results for blocks less than the representative size are not significant.

2. GOVERNING EQUATIONS OF FLOW

Simultaneous gas-water flow is governed by momentum (Darcy's law) and mass balance equations. These equations, being formulated for each phase separately, are coupled through the relationship between phases saturation and through the capillary pressure. To these equations one should add the equations of state, relating the density and the viscosity to pressure and temperature.

(i) Gas flow equations

Darcy's law is

$$u_{gj} = - \frac{k\, k_{rg}(S_w)}{\mu_g} (p_{g,j} - \rho_g g_j) \qquad (1)$$

the mass conservation equation is

$$(\phi \rho_g)_{,t} + (\rho_g u_{gi})_{,i} + Q_g = 0 \qquad (2)$$

where u is specific flux, k is absolute permeability, k_r is relative permeability function of fluid saturation, μ is dynamic viscosity, ϕ is porosity p is pressure, g is the acceleration of gravity and Q is the mass rate of gas production. Subscript g denotes the gas phase.

Expanding the time derivative, one obtains

$$(\phi \rho_g)_{,t} = \phi \rho_{g,t} + \rho_g \phi_{,t} \qquad (3)$$

The density of the gas is related to pressure through the equation of state.

$$\rho_g = \frac{p_g M}{ZRT} \qquad (4)$$

where M is the molecular weight to the gas, R is the universal gas constant, T is temperature and Z is the deviation factor of a real gas from the ideal gas behaviour and is a function of pressure and temperature.

The compressibility of the rock matrix is defined as

$$c_r = -\frac{1}{\phi}\frac{d\phi}{dp} \qquad (5)$$

Substituting the relationships (4) and (5) into (3), we obtain

$$(\phi\rho_g)_{,t} = \frac{\phi M}{ZRT}(1 + p_g c_r)\, p_{g,t} \qquad (6)$$

Substitution of equation (6) together with Darcy's law into equation (2), yields

$$\frac{\phi M}{ZRT}(1 + p_g c_r)\, p_{g,t} - \left(-\frac{k_{rg} k}{\mu_g}\, \frac{p_g M}{ZRT}\left(p_{g,i} - \frac{p_g M}{ZRT} g_i\right)\right)_{,i} + Q_g = 0 \qquad (7)$$

(ii) Water flow equations

Darcy's law is

$$u_{wj} = -\frac{k\, k_{rw}(S_w)}{\mu_w}\left(p_{w,j} - \rho_w g_j\right) \qquad (8)$$

and the equation for the conservation of mass is

$$(\phi\rho_w)_{,t} + (\rho_w u_{wi})_{,i} + Q_w = 0 \qquad (9)$$

where subscript w denotes the water phase.

Expanding the time derivative in equation (9), one obtains

$$(\phi\rho_w)_{w,t} = \phi\rho_w c_w p_{w,t} + \rho_w \phi c_r p_{w,t} = c\rho_w \phi\, p_{w,t} \tag{10}$$

where $c = c_w + c_r$ is the total (water and rock) compressibility. Substitution of equation (10) and Darcy's law into equation (9) yields

$$\phi\rho_w c\, p_{,t} - \left(\frac{k\, k_{rw}}{\mu_w}\rho_w (p_{w,i} - \rho_w g_i)\right)_{,i} = 0 \tag{11}$$

(iii) Phase saturations relationship

As follows from the definition of saturation, for the two phases gas and water, filling the entire pore space

$$S_g + S_w = 1 \tag{12}$$

(iv) The capillary pressure

The pressure in the gas and in the water phase are related through the capillary pressure (p_c)

$$p_c(S_w) = p_g - p_w \tag{13}$$

3. METHOD OF SOLUTION

The V.I.P. computer program is based on a finite difference method of solution to the equations of flow presented in the previous paragraph.

4. INPUT PARAMETERS

4.1 The geometry of the flow domain

The repository is assumed to have a width of 12 metres, a height of 15 metres and a length of 160 metres. It is located at a depth of 50 metres below the sea bottom. The sea water level is 6 metres above the rock formation (Fig. 1).

The flow domain considered is a vertical cross-section passing through the repository. For reasons of symmetry it is enough to investigate only half flow domain with the axis of symmetry passing the centre of the repository. The considered half flow domain has an extent of 328 m in the horizontal direction and of 345 m in the vertical direction.

The flow domain was discretized into a quadrilateral grid of 18 blocks in the horizontal direction and 23 blocks in the vertical direction resulting in a total number of 414 grid blocks. The grid increments in the horizontal and in the vertical directions are presented in Table 1 and 2, respectively.

Table 1: Grid increments in the horizontal direction *)

Block number	1	2	3	4	5	6	7	8	9
Increment (m)	3.0	1.5	0.8	0.4	0.2	0.1	0.1	0.2	0.4

Table 1 (continued)

Block number								
10	11	12	13	14	15	16	17	18
Increment (m)								
0.8	1.5	3.0	6.0	10.0	20.0	40.0	80.0	160.0

Table 2: Grid increments in the vertical direction *)

Block number											
1	2	3	4	5	6	7	8	9	10	11	12
Increment (m)											
10	10	9	9	6	3 1	.5	.8	.4	.2	.1	.1

Table 2 (continued)

Block number										
13	14	15	16	17	18	19	20	21	22	23
Increment (m)										
.2	.4	.8	1.5	2.5	4.0	5.5	5.5	10.	22.	40.

*) In the horizontal directions the grid blocks are numbered from the left to the right; in the vertical direction the grid blocks are numbered downwards

4.2 Rock and fluids parameter values

Rock and fluid parameters values are indicated in Table 3. Reference values are adjusted to the prevailing pressure and temperature conditions by the V.I.P. program.

Table 3: Parameter values

Parameter	Symbol	Value	Units
rock permeability	k	$5.28*10^{-15}$	m^2
porosity		10^{-4}	
capillary pressure	p_c	Fig. 3	Pa
relative permeabilities	k_r	Fig. 4	-
compressibility of water (reference value)	c_w	$4.57*10^{-6}$	kPa^{-1}
rock compressibility	c_r	$6.10*10^{-6}$	kPa^{-1}
density of water (reference value)	ρ_w	1000.	kgm^{-3}
dynamic viscosity of water	μ_w	$1.0*10^{-3}$	Pas
density of the gas	ρ_g	$\rho_g = \frac{p_g M}{ZRT}$	kgm^{-3}
dynamic viscosity of the gas (reference value)	μ_g	$8.5*10^{-6}$	Pas
molecular weight of hydrogen	M	2.016	$kg\ mole^{-1}$
universal gas constant	R	8.3143	$J\ mol^{-1}K^{-1}$
temperature	T	283.16	K
deviation factor for real gases	Z	$Z = Z(p,T,M,R)$	-

5. BOUNDARY AND INITIAL CONDITIONS

The upper boundary, corresponding to the sea bottom is a constant pressure boundary. A pressure of 160.125 kPa, corresponding to a water column of 6 metres, was imposed on this boundary. The other boundaries (Fig. 2) are considered no flow (impervious) boundaries. The reason for this is that the left hand side boundary passing through the repository is a streamline, while the other boundaries are considered to be located far enough from the repository, so that the conditions imposed on these boundaries are not affected by the local flow phenomena in the region of the repository.

Such conditions correspond to an isolated cavern or to a system of parallel cavern located far enough from each other so that flow phenomena not interfere. The boundaries of the cavern are assumed pervious and not affected by the operations during the excavation.

The rate of production of gas resulting from corrosion is estimated to be 20000 normal cubic metres per year. This rate of flow distributed over the length of the cavern of 160 m, results in a rate of 0.34 normal cubic metres per day and metre. In the model this rate of flow was generated by distributed sources in the two-dimensional cross section of the cavern.

After filling the cavern the initial conditions of the flow through the aquifer will be reestablished. Neglecting the natural flow through the aquifer, these conditions correspond to a hydrostatic pressure distribution. This water pressure distribution and fully water saturated medium (S_w) were considered to be the prevailing initial conditions (Fig. 8).

6. RESULTS

The results of the calculations, the saturation distribution at different times of displacement and the pressure distribution at breakthrough, are presented in Figs. 5 to 8.

In the empty cavern the gas formed in the cavern moves almost instantaneously upward and accumulates below the roof of the cavern. The gas penetrates the rock and displace water after a gas cushion of 0.4 m, corresponding to the assumed entry capillary pressure value, is formed below the roof of the cavern.

In the cavern, during the all stages of displacement, the gas-water interface is absolutely horizontal and differs from Intera results with a slope of the interface increasing from the centre of the repository outward.

The saturation distribution and the gas-water front ($S_w = 1$) at the different stages of displacement, up to the breakthrough time equals to 0.6 days, is presented in Figs. 5 to 7. The gas advance, faster in the centre of the repository and slower at the edges, this way consistent to the expected physical behaviour. It differs from the results obtained by Intera with a faster advance at the edges of the repository and almost stagnant in the centre.

The breakthrough time at the sea bottom is 0.6 days in comparison to 11 days obtained by Intera.

Because of the large difference in the gas-water densities the displacement is limited to the near region to the repository. This means that the obtained results are relevant for a single cavern with lateral boundaries far for the repository, as well as for a system of parallel caverns located at a distance say two times the width of the cavern.

Pressure increases gradually in the cavern and reaches its highest value just before the breakthrough of the gas at the sea bottom. The present study indicates a maximum pressure increase in the cavern of 28.2 kPa. Intera reports an increase in the pressure in the cavern of 62 kPa after 2 days. That is to say considerably before the stated breakthrough time when the pressure is likely to have been much higher than after only 2 days.

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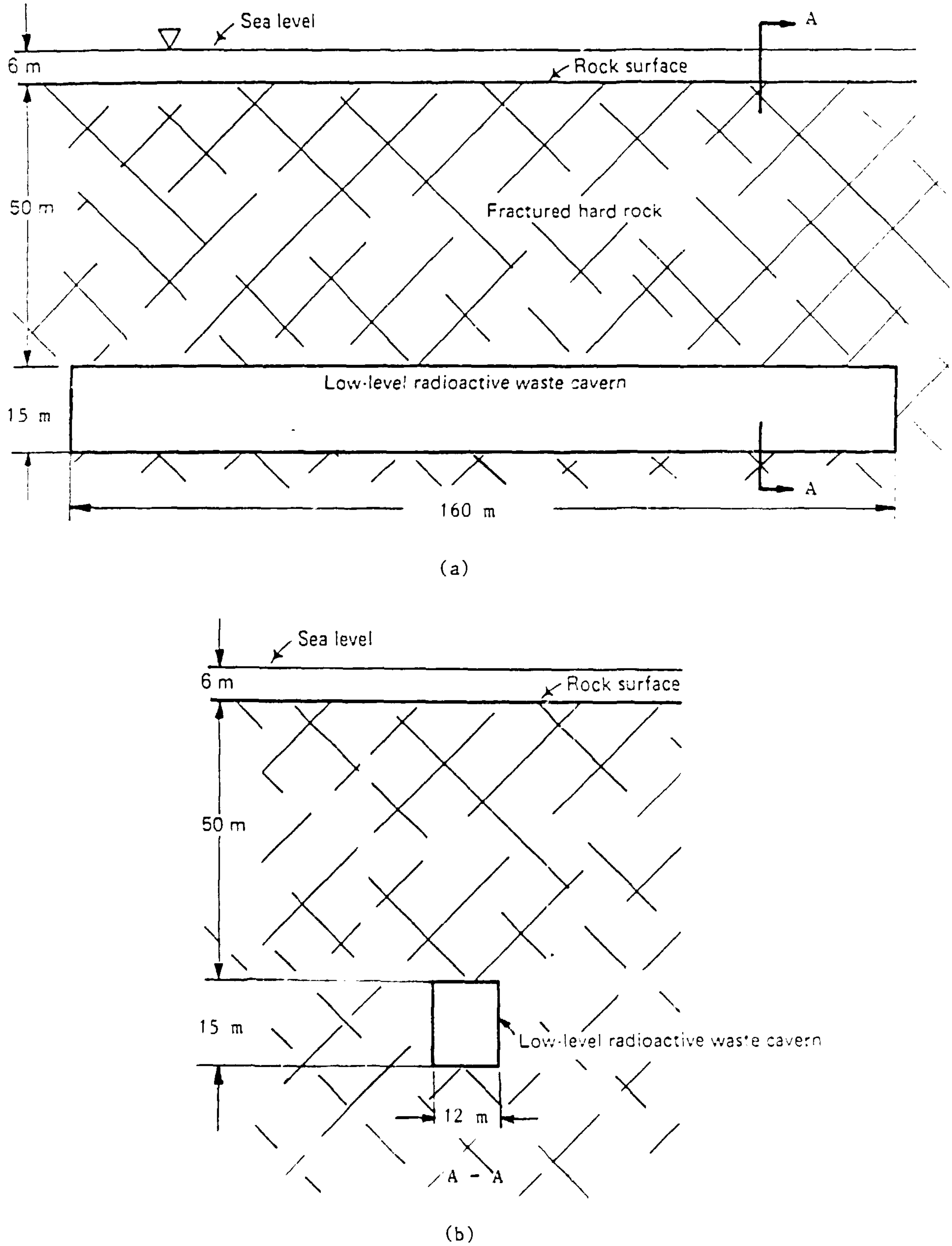
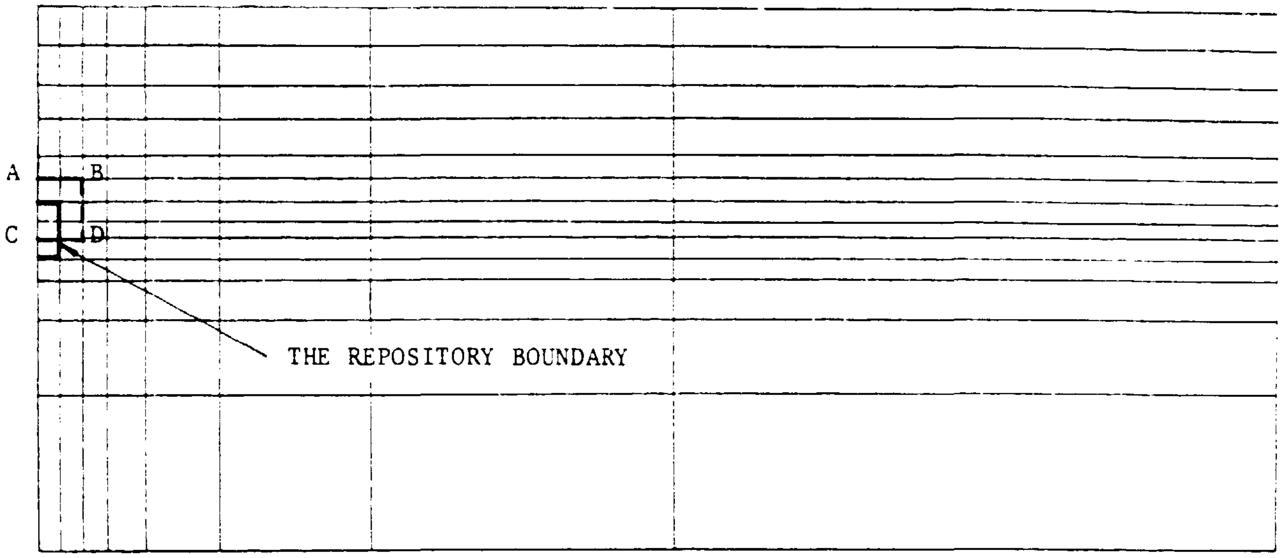
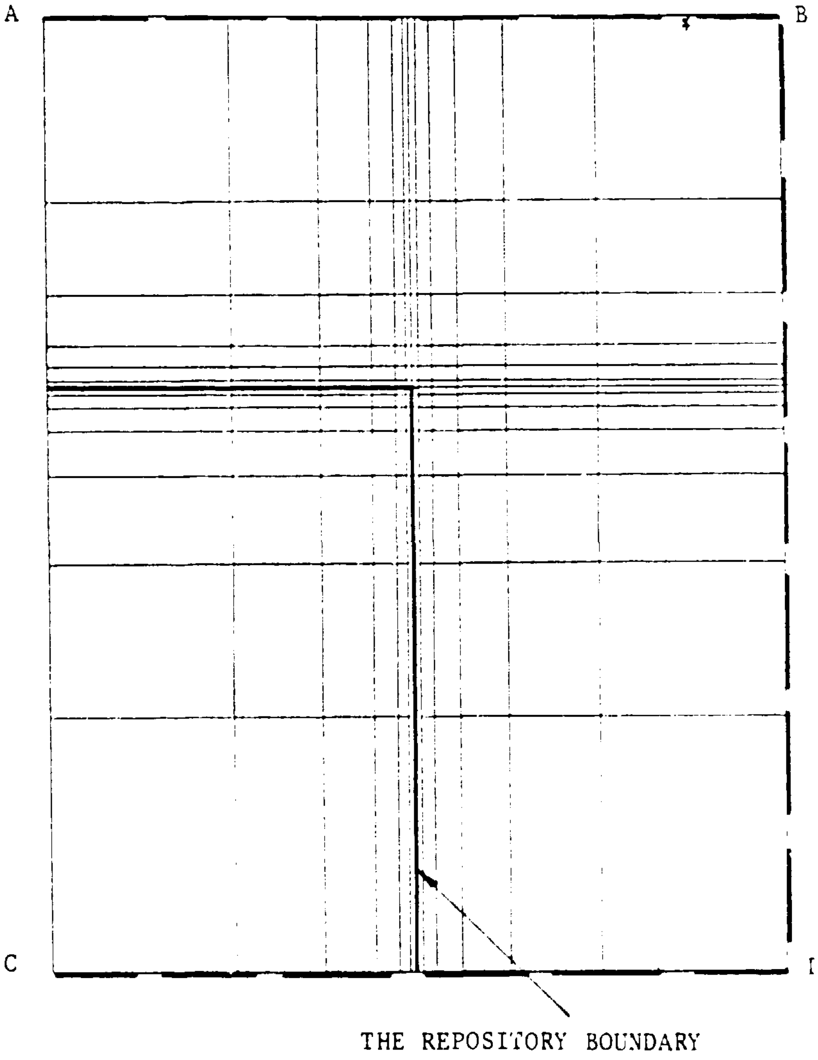


Figure 1. Schematic representation of the location of the repository: (a) a longitudinal cross-section and (b) a transverse cross-section through the repository.



(a)



(b)

Figure 2. The discretization of the flow domain: (a) total flow domain and (b) the region around the repository.

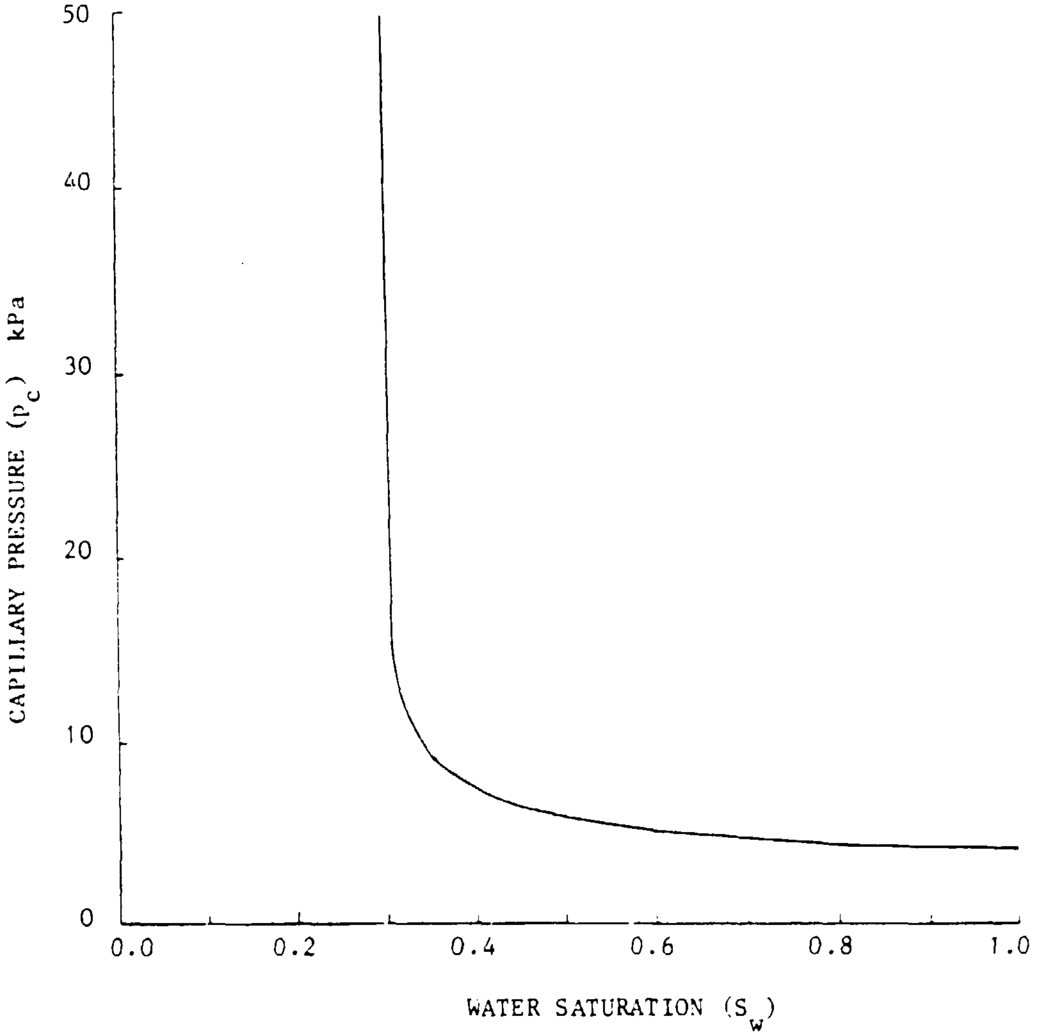


Figure 3. The capillary pressure function of saturation.

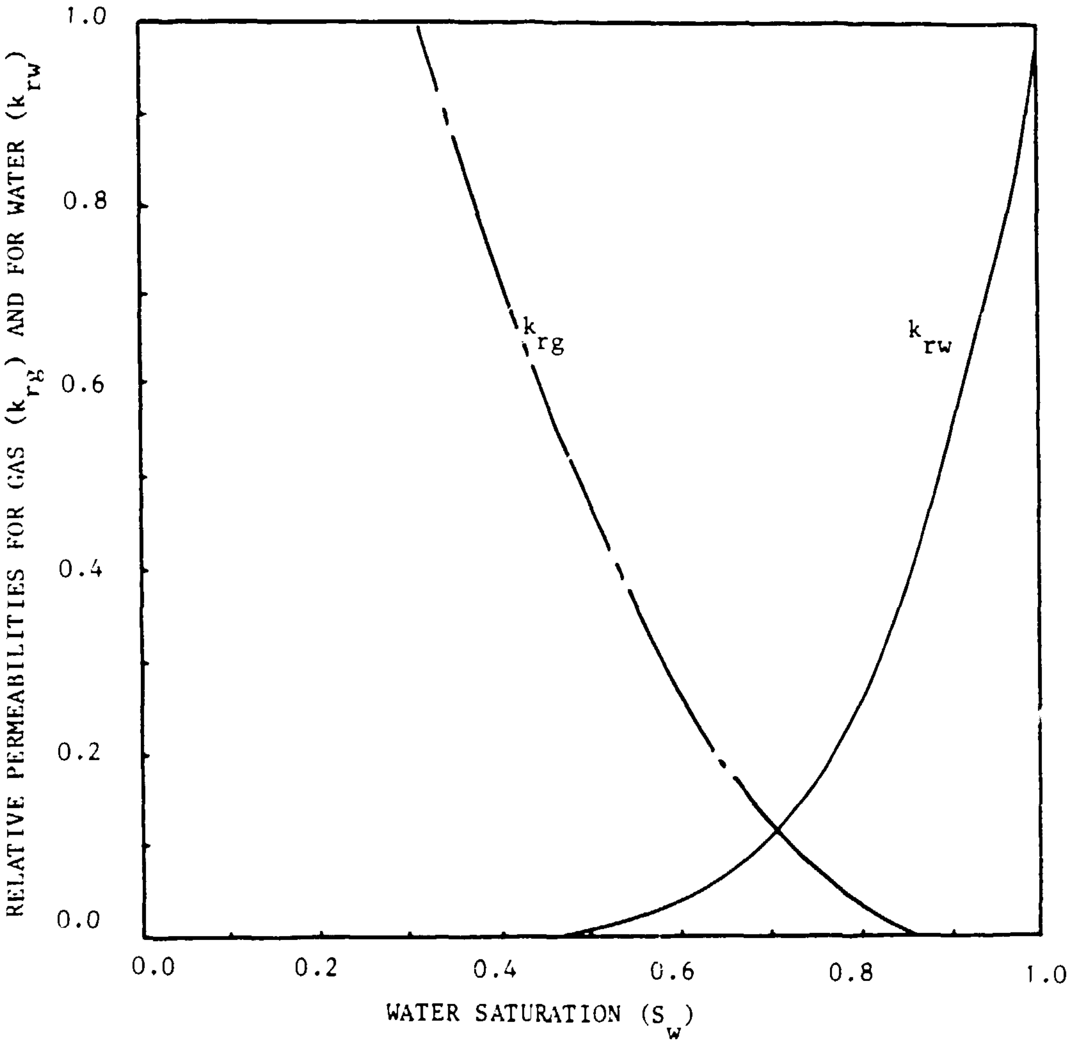


Figure 4. The relative permeabilities for gas and water as functions of saturation.

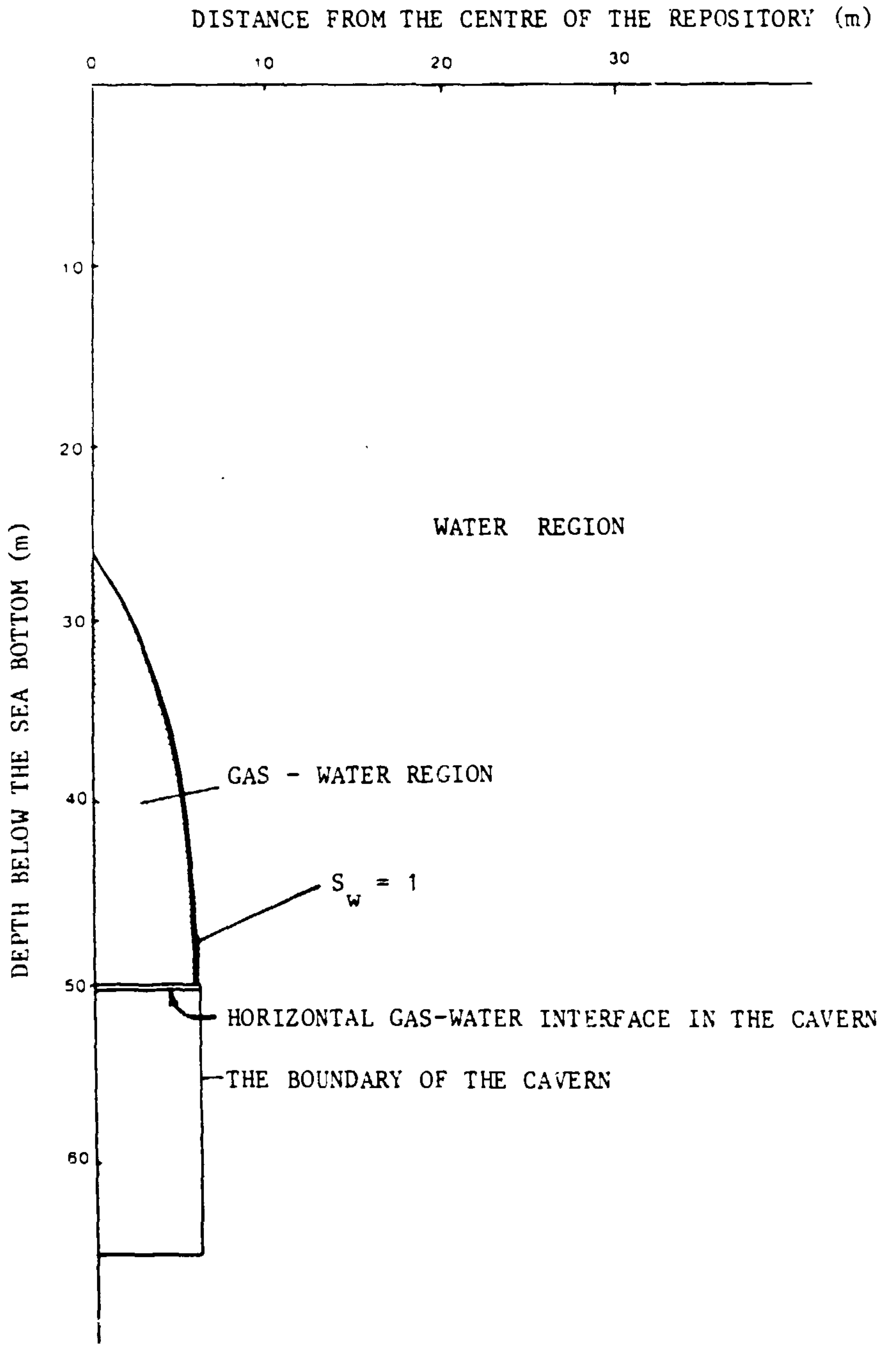


Figure 5. The gas-water front after 0.45 days.

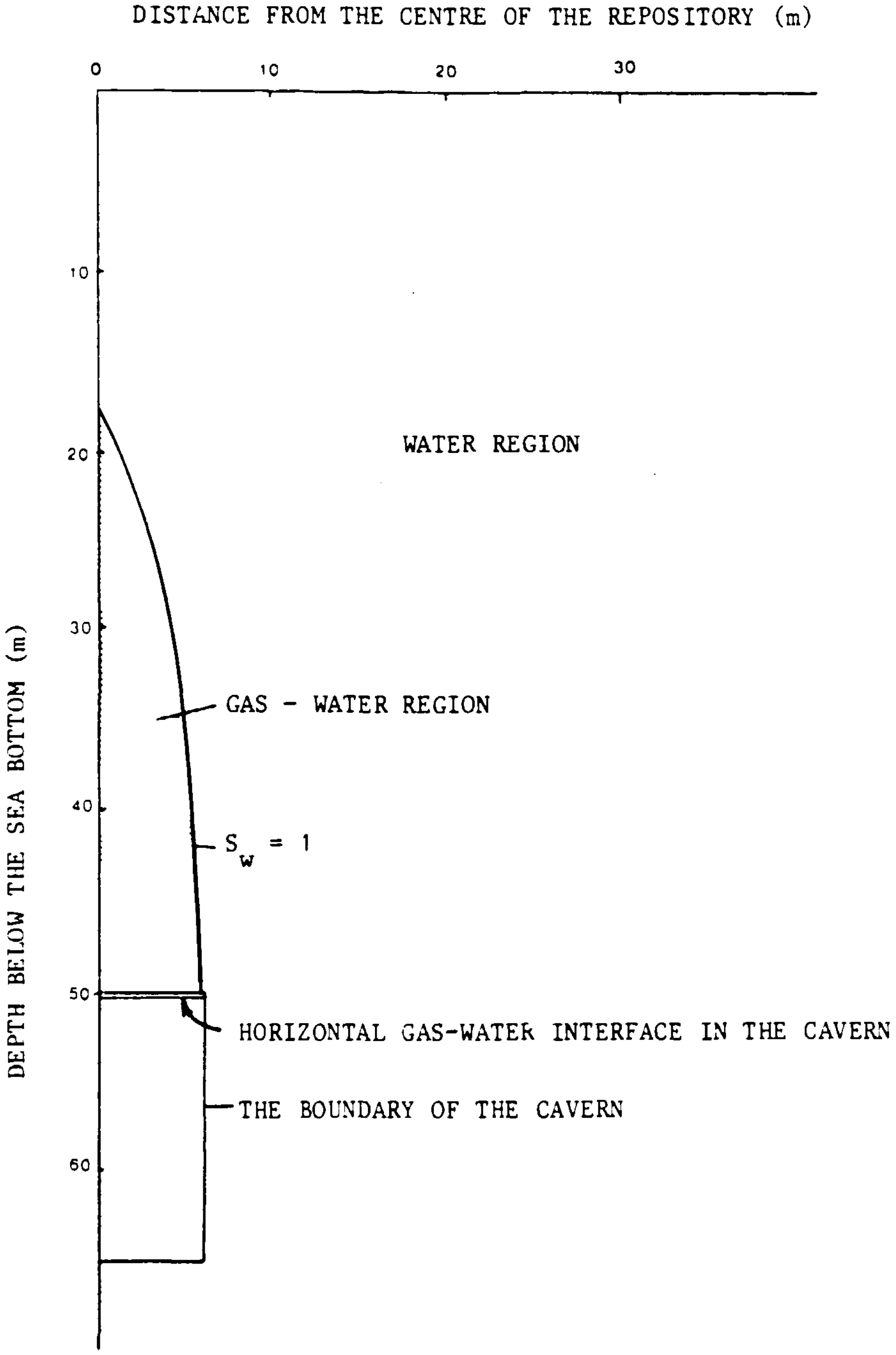


Figure 6. The gas-water front after 0.55 days.

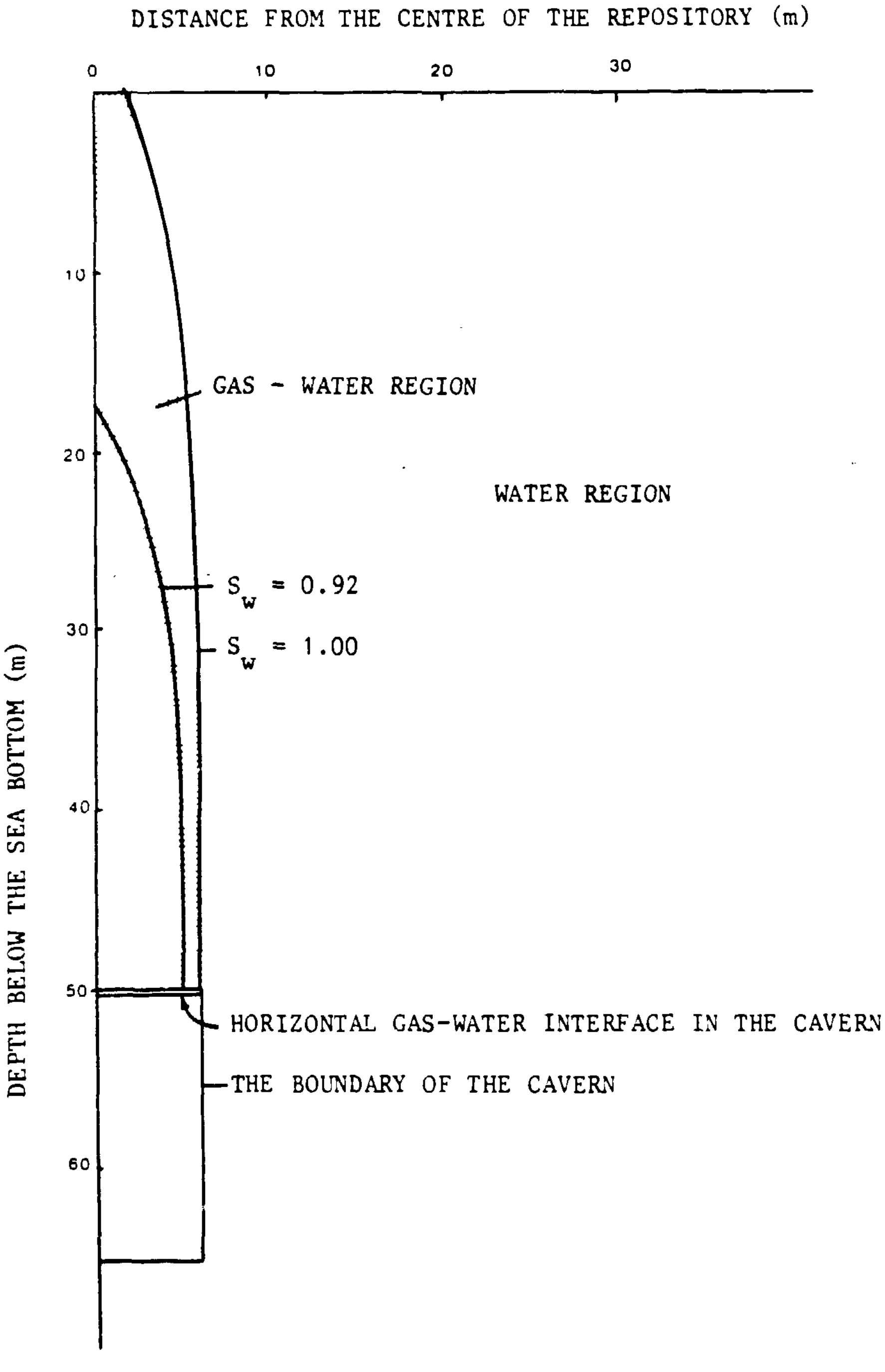


Figure 7. The gas-water front and the water saturation distribution at breakthrough at 0.6 days.

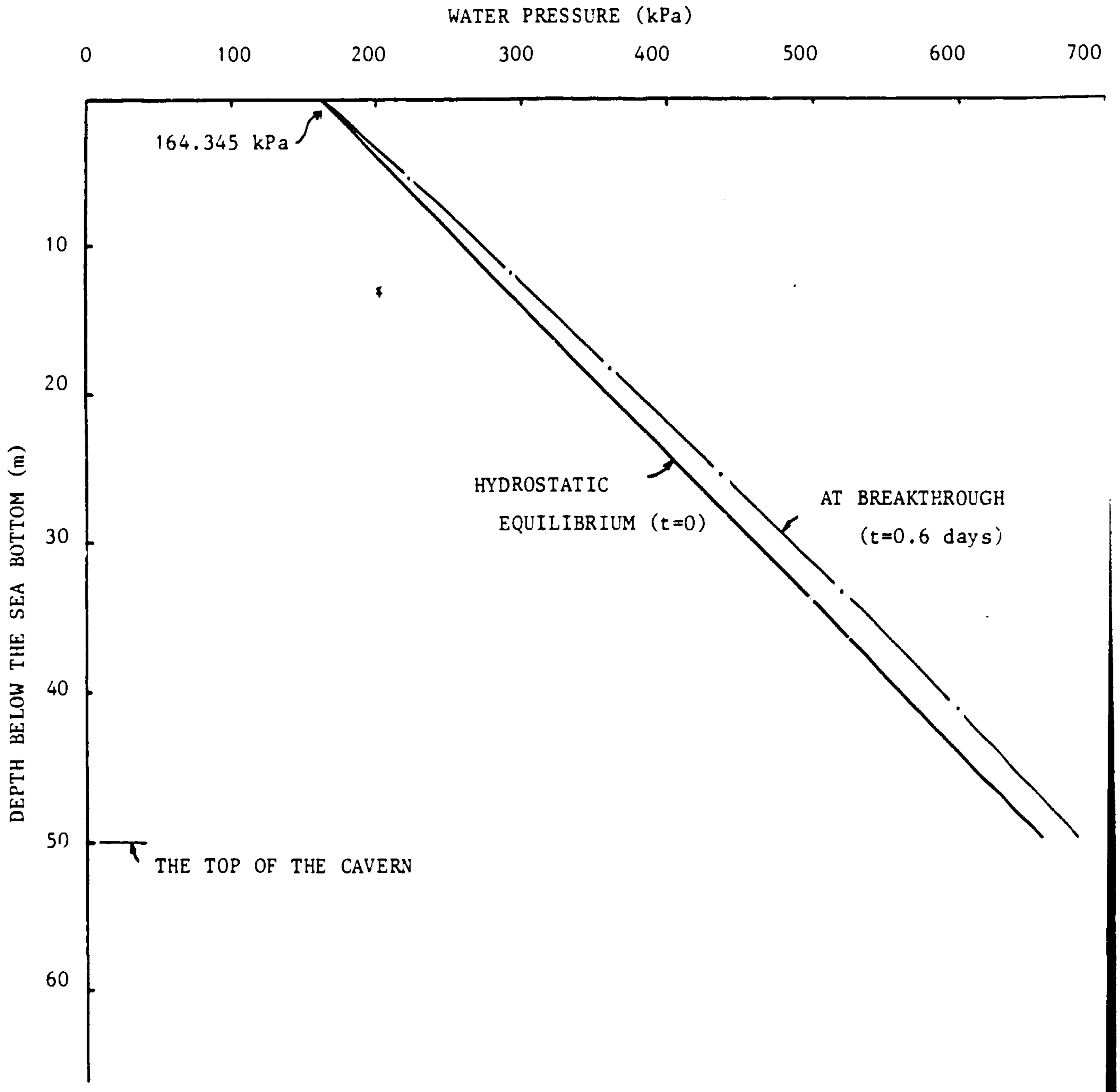


Figure 8. The initial (hydrostatic water pressure distribution and at the breakthrough at 0.6 days.

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