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A numerical simulation of the origin and composition of the groundwater below Äspö

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Computer-aided Fluid Engineering AB

Februari 1999

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ABSTRACT

An attempt is made to calculate the origin (in the time and space) of the waters found below Äspö. It is assumed that the present water composition is due to the conditions prevailing after the last glaciation (initial conditions) and the hydrological events after this time (resulting in transient boundary conditions). The total time span simulated is from 10 000 years BP (Before Present) to 5 000 years AP (After Present).

The different water types are tracked by solving an advection/diffusion equation for each of the identified water types. This novel technique is called the 'fluid population method' and is a simple and straightforward computational technique.

Results from the simulation include the distribution of different water types in space and time and some detailed results for the conditions at 450 metres below Äspö (water composition, transport time to ground level).

The main conclusion from the study is that the simulation model gives plausible results. However, the uncertainties about the basic conceptual model and the boundary conditions do not presently make a direct comparison with field data meaningful.

ABSTRACT (Swedish)

Ett försök görs att simulera vattnets ursprung och sammansättning under Äspö. Ett grundläggande antagande är att nuvarande vattensammansättning är ett resultat av förhållandena efter senaste istiden och de hydrologiska förhållandena efter denna tidpunkt. Totalt simuleras en period som sträcker sig från 10 000 år BP (Before Present) till 5 000 år AP (After Present).

De olika vattentyperna spåras med hjälp av ett antal advektions/diffusions ekvationer; en för varje identifierad vattentyp. Tekniken kallas "the fluid population method" och är en enkel och lätt implementerad beräkningsmetod.

Som resultat av simuleringen erhålls fördelningen, i rum och tid, för varje identifierad vattentyp. Speciellt studeras förhållandena på 450 meters nivå under Äspö (vattnets sammansättning, transporttid till marknivå).

Slutsatsen av arbetet är att den formulerade beräkningsmodellen ger rimliga och förväntade resultat. Osäkerheten rörande grundläggande antaganden och randvärden är emellertid betydande och direkta jämförelser med fältmätningar är för närvarande inte meningsfulla.

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1 INTRODUCTION

As general background to the work to be described we may cite the following paragraphs from Wikberg (1998):

> Groundwater flow models are used to describe the slow transport of groundwater from recharge areas down through the deep geological formation and then back to discharge areas where it eventually reaches the biosphere. Groundwater changes its composition along the flow path. The concentration of dissolved salts generally increases with depth and relative amounts of dissolved components changes. Recharging oxygen is depleted and the pH is stabilised. These changes are not described by groundwater flow models.
>
> The distribution of the flow at repository level and the transport time from the repository back to the biosphere are essential for the calculations of nuclide migration from a leaking waste canister. The chemical composition of the groundwater is also needed to calculate the dissolution rates, concentrations and retardation of the hazardous radionuclides.
>
> The composition and evolution of the groundwater chemistry is a result of reactions between the groundwater and rock minerals and mixing of groundwater of different origin. Therefore, it is of interest to combine groundwater travel time and flowpaths with the groundwater chemistry. However, this is difficult because the mixing of groundwater that dominates the presently observed conditions and which to a large extent is a result of previous varying hydraulic (boundary) conditions.

The objective of this study is to make a first attempt to calculate the groundwater composition (with respect to origin) below the island of Äspö. It needs to be emphasised that the study is a feasibility study as we are not considering chemical reactions nor mixing of waters of different origin.

The computational domain is shown in Figure 1-1. The domain is the same as used in the regional model presented in Svensson (1997). Actually, this regional model forms the starting point for the present investigation and the reader is referred to the report for details about the model formulation, calibration exercises, etc. A major difference from the regional model is that the present simulation is transient covering a period from10 000 years BP (Before Present) to 5 000 years AP (After Present).

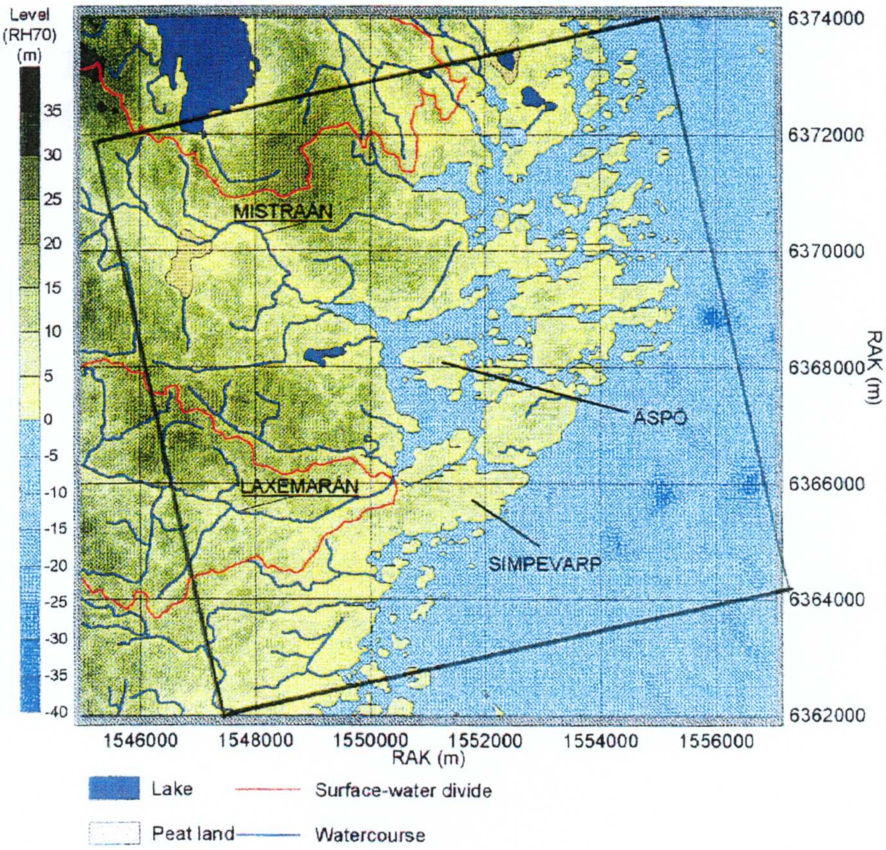

Figure 1-1. *The area considered in the model. The black square indicates the model area (10 x 10 km^2) oriented in the Äspö coordinate system.*

During the period 0 → 10 000 years BP the sea level and salinity of the Baltic have varied considerably, while conditions can be expected to be less dramatic during the next 5 000 years. In Figure 1-2 the sea level and salinity during the period are shown and the names of the different stages of the Baltic are introduced. The assumed recharge (precipitation minus evapotranspiration) is also given in Figure 1-2. The present recharge has been estimated to 200 mm/year, but the variation during the last 10 000 years is harder to estimate. It is however known that the mean temperature was a few ^{0}C higher 5 000 years BP which may reduce the recharge. During the next 5 000 years one can expect a decrease in temperature, which may increase the recharge. Based on these considerations the variation given in Figure 1-2 was estimated.

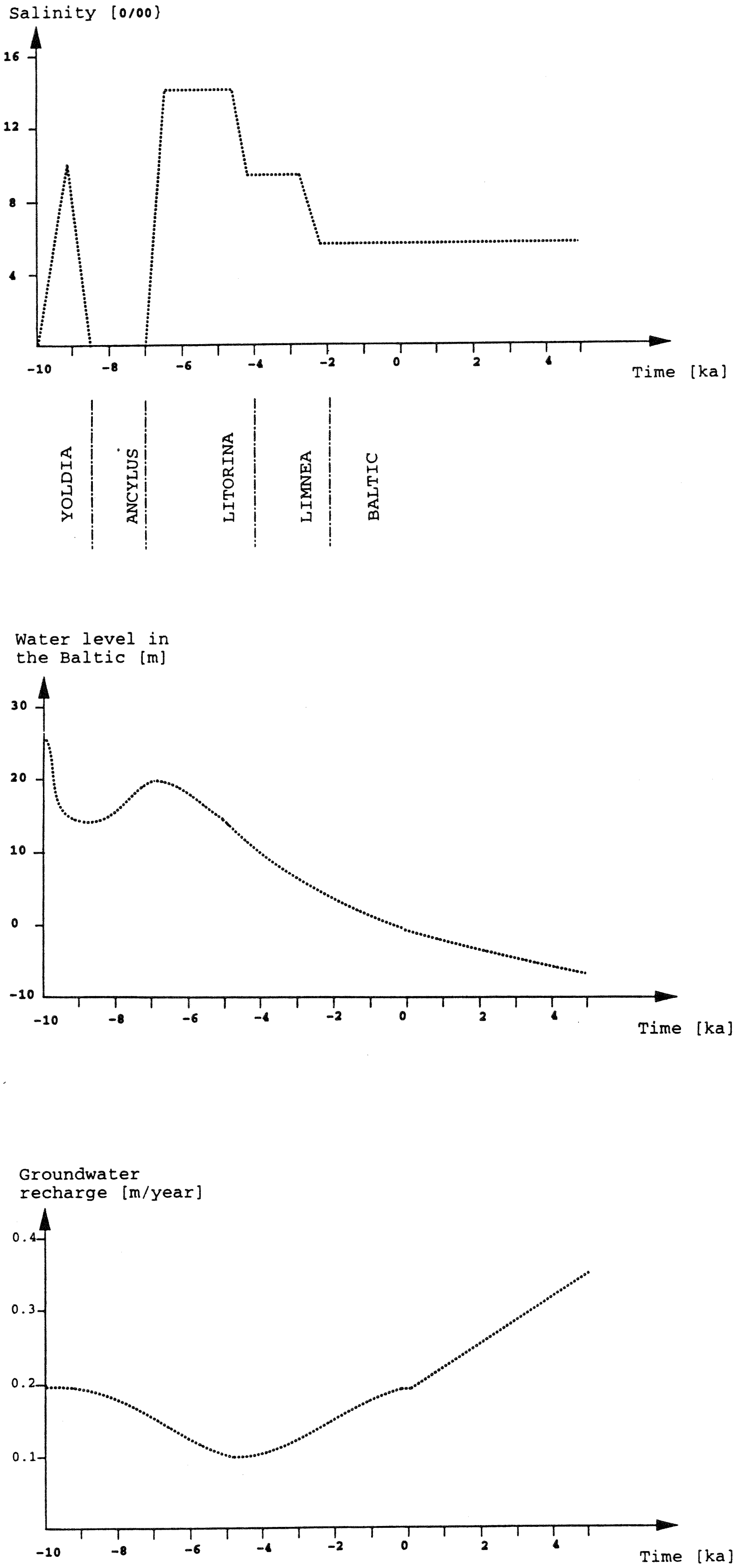

Figure 1-2. *Assumed boundary conditions for the period 10 000 years BP to 5 000 years AP.*
Top: Salinity variation (after Westman (1997)).
Middle. Water level in the Baltic (after Påsse (1996)).
Bottom: Groundwater recharge.

2 BASIC CONCEPTUAL ASSUMPTIONS

The simulation model to be presented in this report rests on one major assumption that can be formulated as follows:

- The water composition 500 metres below Äspö is determined by the conditions prevailing after the last glaciation (initial conditions) and the hydrological events after this time (resulting in transient boundary conditions).

This basic statement needs to be elaborated upon. From field measurements (Laaksoharju et al (1995)) it is known that the water below 800-1 000 metres depth is almost stagnant; it has often been quiescent as long as our dating techniques can determine. This water was hence there when the last glaciation ended (about 12 000 years BP) and is still there. Our simulations can accordingly not say anything about the conditions below a depth of, say, 800 metres and this is the reason why we restrict ourselves to 500 metres in the statement above. It is however essential to represent the dense stagnant layer below 800 metres in the model. This is done by the initial conditions.

The present water composition is further assumed to be due to the hydrological events during the last 10 000 years. In the simulations the water level and salinity of the Baltic and the freshwater recharge on land are considered. Mixing and chemical reactions are not taken into account. As mentioned in the previous chapter the Baltic Sea has had a variation in salinity over the last 10 000 years. The basic idea of the simulations is to track the water from the different periods of the Baltic, as identified by the salinity variations, by marking the water as it enters the domain through the upper boundary. We can of course also mark the water we have initially in the domain and the recharge water on land. These different water types are sometimes called end-members (Laaksoharju (1997)) as they constitute the possible sources of mixed water found somewhere in the rock. The ultimate goal of the simulations is to compare the predicted water composition with the end-members found in field measurements. There are however several reasons why this comparison, at the best, can only be qualitative. Above it was mentioned that we neglect mixing and chemical reactions which of course is a gross simplification. Another simplification is that we neglect storage of water in stagnant parts (cavities, dead-end fractures, etc) of the rock. To take this process into account a double-porosity technique is required; this is however not within the reach of this project as it would require some development work and significantly more computer power.

Coming back to the basic assumption above, it was stated that hydrological events during the last 10 000 years govern the present water composition below Äspö. Above we excluded mixing and chemical reactions and we also need to exclude large scale regional influences, if such exist. However, from the centre of Äspö the horizontal distance to the vertical boundaries is 5 km and it is likely that the variations in the upper boundary conditions influence the conditions below Äspö more than regional influences.

In Figure 2-1 the exchange of water at various stages of the Baltic is illustrated. The vertical section shown can be thought of as an east-west section through Äspö. The location of the fresh-salt water interface is governed by the Ghyben-Hertzberg relation. If the sea water salinity changes the position of the interface changes and large volumes of water are displaced. Note that the salt water below 1 000 metres is not expected to move and hence provide a lower boundary for the exchange of water. At about 4 000 years BP Äspö became an island and a fresh water lens below Äspö was established. This lens, and in particular its depth, can also be expected to vary with the sea water salinity and hence generates displacement of water. Another strong mechanism for water exchange is unstable density stratification. When the sea water salinity increases we get heavier water on top of lighter; a situation that will induce a strong vertical exchange of water (free convection or density overturning).

For the period 0 $\rightarrow$ 5 000 years AP, the boundary conditions are even more uncertain. If however the water level in the Baltic drops as shown in Figure 1-2, we also need to consider what happens when Äspö becomes an island in a freshwater lake. This will of course happen when the water level in the Baltic drops below the sill level in the deepest connection to the Baltic, see Figure 2-1. One can expect that this sill level is 2-3 metres below the present level of the Baltic and, according to Figure 1-2, the transition will then happen at 2 000 $\rightarrow$ 3 000 years AP. After this time it will be assumed that Äspö is an island in a freshwater lake, with a water level of 2-3 metres below present level.
These are the main ideas and assumptions about the physical processes believed to be significant for the situation studied.

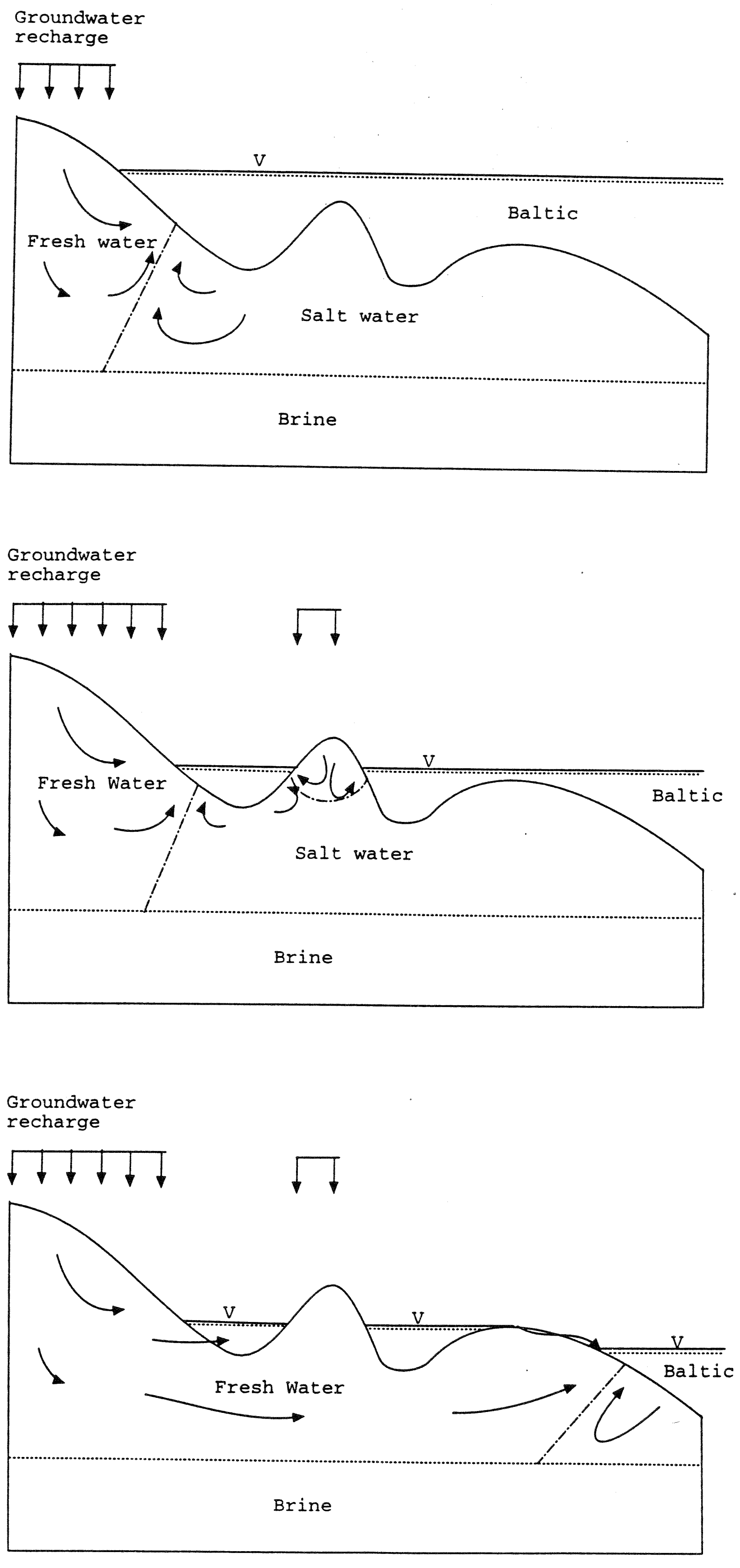

Figure 2-1. *Schematic figure of water exchange at different stages of the Baltic Sea.*

- *Highest point on Äspö below sea level (top).*
- *Äspö is an island in the Baltic Sea (middle).*
- *Äspö is an island in a freshwater lake (bottom).*

3 MATHEMATICAL MODEL

3.1 BASIC APPROACH AND ASSUMPTIONS

Groundwater models can be developed for a number of purposes; perhaps the most common one is that the rainfall - runoff relation is requested. As stated above, the objective of the present study is to understand the development of the groundwater composition below the island of Äspö. With this in mind the following basic requirements for the simulation model have been formulated:

- It needs to be transient and three-dimensional with high resolution in space.

- Variable density needs to be accounted for, as the salinity of the groundwater will vary in time and space.

- The model should predict a realistic groundwater level, as we expect a balance between the pressure generated by the water table and the pressure due to the internal density distribution.

We will further introduce some basic assumptions; some of which are motivated by the purpose of the study, others by the lack of information or data. The following assumptions are made:

- Spatial uniformity. Due to lack of data we need to assume that precipitation and evapotranspiration are horizontally uniform. Variations in vegetation and soil types are also neglected.

- The unsaturated zone can be handled by the simple algorithm introduced in Svensson (1995).

The computational domain was introduced in Figure 1-1. The motives for the size and orientation of the domain can be summarised as follows:

- The orientation should follow the Äspö coordinate system, for simple and secure integration with the Äspö data base.

- The computational grid should not have more than 400 000 cells, in order to avoid extreme execution times on a low-end workstation.

These considerations led to a domain of 10 x 10 x 3 km^3, centred around the Äspö HRL, represented in a computational grid of 100 x 100 x 36 cells.

These are the basic requirements and assumptions of the model.

3.2 GOVERNING EQUATIONS

For the momentum balance it will be assumed that the Darcy law applies. This means, among other things, that the time derivative is neglected.

With this assumption, and the ones in the previous section, the following set of equations can be formulated.

Momentum:

$$0 = -\frac{\partial p}{\partial x} - \frac{\rho g}{K_x} u \tag{1}$$

$$0 = -\frac{\partial p}{\partial y} - \frac{\rho g}{K_y} v \tag{2}$$

$$0 = -\frac{\partial p}{\partial z} - \frac{\rho g}{K_z} w - \rho g \tag{3}$$

Salinity balance:

$$n\frac{\partial s}{\partial t} + \frac{\partial}{\partial x} us + \frac{\partial}{\partial y} vs + \frac{\partial}{\partial z} ws = \frac{\partial}{\partial x}\left(D\frac{\partial s}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial s}{\partial y}\right) + \frac{\partial}{\partial z}\left(D\frac{\partial s}{\partial z}\right) \tag{4}$$

Mass balance:

$$\frac{\partial}{\partial x}\rho u + \frac{\partial}{\partial y}\rho v + \frac{\partial}{\partial z}\rho w = 0 \tag{5}$$

Equation of state:

$$\rho = \rho_0 (1 + \alpha\, s) \tag{6}$$

Where *u, v, w* are Darcy velocities, *p* pressure, *s* salinity (in %, by weight), K_x, K_y, K_z conductivities, *D* hydraulic dispersion coefficient, *n* kinematic porosity $(= 10^{-3})$, α a coefficient $(= 7.41 \times 10^{-3})$, ρ_0 a reference density of water (= 1 000 kg/m^3), ρ density of water and g gravitational acceleration. The coordinate system is denoted *x, y, z* with *x* in the east direction, *y* north and *z* vertical upwards.

It is still unclear (at least to the author) how the hydraulic dispersion coefficient ought to be interpreted and determined in a fractured rock. For a general porous media, where a representative elementary volume can be defined, general tensor expressions are available, see Bear et al (1987). A further complicating factor is that we are going to apply the salinity equation in a discretized form, i.e. on our computational grid. A suggestion is that the dispersion coefficient should account for sub-grid mixing processes. Due to the uncertainty about the interpretation of the process we will assume that the dispersion coefficient is isotropic, proportional to the local velocity and the grid-size, hence:

$$D = \beta\Delta|\vec{U}| \tag{7}$$

where β is an unknown coefficient, Δ the grid-spacing and $|\vec{U}|$ the magnitude of the Darcy-velocity. As seen, the effect of molecular diffusion is also neglected in (7). A constant value of 10 metres was set for the product $\beta\Delta$.

In order to track the various components of the groundwater an advection/diffusion equation is solved for each component:

$$n\frac{\partial c_i}{\partial t} + \frac{\partial u_j c_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D_c \frac{\partial c_i}{\partial x_j}\right), \qquad \mathrm{i} = 1, \mathrm{k} \tag{8}$$

where c_i is the marker for water type *i*. We will not consider dispersion effects in the present context and D_c is hence zero. To track the component that originates, say, from 8 000 to 7 000 BP (Before Present), we put the upper boundary condition to 1.0 for relevant *c*-variable. The initial condition for the *c* is zero, which is also the boundary value for all other time intervals. To track the brine-water we put the relevant *c*-variable to 1.0 below, say, 800 metres as an initial condition and use a zero-flux condition at all boundaries at all times.

3.3 GEOMETRIC FRAMEWORK AND MATERIAL PROPERTIES

The major transmissive fracture zones in the region are shown in Figure 3-1. The transmissivities have been estimated, see Rhén et al (1997), to be 0.3×10^{-5} m²/s (W) and 10.0×10^{-5} m²/s (WW). Hydraulic conductivities at different depths for the rock inbetween the fracture zones have been estimated from field measurements, see Rhén et al (1997). It is well-known that these conductivities, and their standard deviations, vary with the testscale. When a numerical model is set-up one needs to consider the relation between the cell size in the grid and the testscale. The values given in Table 3-1 represent a testscale of 100 metres, which is also the cell size in the numerical model. The values for depth > 600 metres are however strictly for a testscale of about 300 metres. For further details about scaling laws and details about the field measurements, see Rhén et al (1997).

Table 3-1. Rockmass hydraulic conductivity and its standard deviation for the region considered. After Rhén et al (1997).

Depth (m)	K (m/s)	s ($\log_{10}$ K)
0 - 200	1.3 E-7	0.96
200 - 400	2.0 E-7	0.65
400 - 600	2.6 E-7	0.79
600 →	4.7 E-8	0.72

The computational domain is $10 \times 10 \times 3$ km^3, which is represented in a grid with a total of 360 000 cells $(100 \times 100 \times 36)$. Part of the grid is shown in Figure 3-2. As can be seen the grid follows the topography (boundary-fitted grid), but has a uniform cellsize (= 100 metres) in the horizontal plane. The vertically non-uniform grid is restricted to the top 100 metres of the domain. For this part of the grid we start with a cellsize distribution (from groundlevel downwards) as follows: 1, 2, 4, 8, 15, 25 and 45 metres. This sequence of cells is then stretched/compressed to follow the topography, which means that the cell-sizes in the sequence are somewhat smaller below the Baltic and somewhat larger below land. Below 100 metres the cellsize is 100 metres in all three directions. It should be noted that the grid follows the sea-bed and not the free surface of the Baltic.

Conductivities for the top four cell layers, i.e. down to 15 metres, are given a special interpretation. One reason for this is that the soil cover can be expected to have a conductivity which is high, but rapidly decreasing with depth. Another is that small ephemeral rills and channels need to be accounted for by the conductivity of the near ground surface cells. The two major rivers in the domain, Mistraån and Laxemarån, are however accounted for by marking the relevant surface cells and give these a significantly higher conductivity. The flow in the rivers is about 0.1 m^3/s and the cross area of the surface cell is 1 x 100 m^2. Using these data it can be shown that putting the conductivity in the "river cells" to 1.0 m/s gives a hydraulic gradient of 10^{-3}, which seems reasonable. The conductivity of the marked river cells is thus put to 1.0 m/s, while the conductivities of the top four cell layers are considered as calibration parameters. Conductivities below the top four layers are generated with the procedure outlined in the next section.

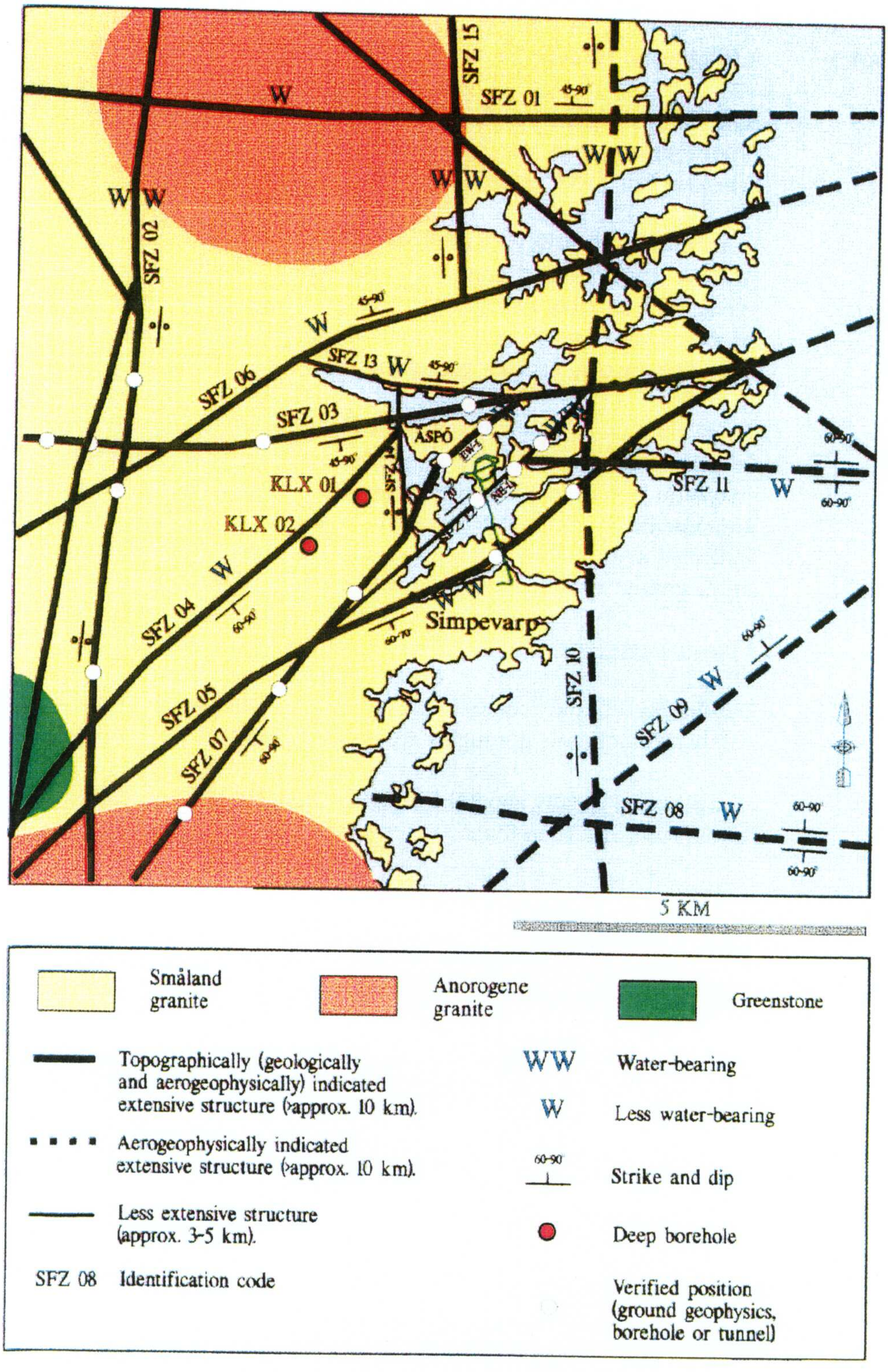

Figure 3-1. Major fracture zones in the area, after Rhén et al (1997).

In Svensson (1997) the conductivities for the top four layers were found to be (from ground downwards) 2.0×10^{-3}, 8.0×10^{-4}, 5.0×10^{-6} and 1.0×10^{-6} m/s. These conductivities are applied horizontally uniformly, which means that we have the same conductivity set below the Baltic Sea as on land.

A further modification of the conductivity field and fracture zone transmissivities is needed to account for unsaturated conditions. A method to predict the depth of the unsaturated zone was introduced in Svensson (1995). Here a brief account of the basic idea of the method will be given.

- Neglect capillary forces, which means that the pressure in the unsaturated zone will be equal to the atmospheric pressure (set to zero).

- The unsaturated zone is partly blocked by air and hence provide higher resistance to flow. Introduce a resistance factor, ϕ, in the balance of forces. The vertical balance, equation (3), then reads:

$$0 = -\frac{\partial p}{\partial z} - \frac{\rho g}{K_z} w\phi - \rho g \qquad (9)$$

- For $\phi = 1$ a negative pressure is predicted for the unsaturated zone. The problem is to find a ϕ - field that gives zero pressure in the unsaturated zone and, of course, has a value of 1.0 in the saturated zone. This can be achieved by an iterative procedure, see Svensson (1995) for details and applications.

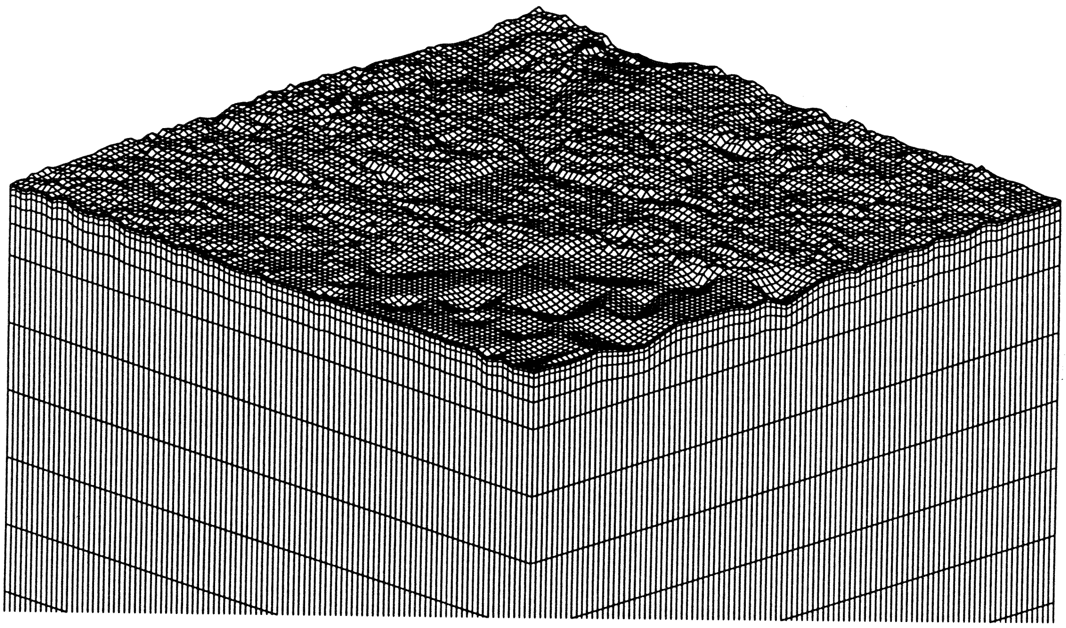

Figure 3-2. *Computational grid close to ground. 100 metres below sea level a uniform grid is used. The vertical scale has been stretched in the figure. View from south-east.*

3.4 SPATIAL ASSIGNMENT METHOD

The conductivity and transmissivity data given in the previous section need to be assigned to the computational grid. The main steps in this procedure are:

- Generate a conductivity randomly for each computational cell using the geometric mean values and standard deviations given in Table 3-1. No correlation is assumed between the cells.

- Generate cell wall conductivities by calculating a geometric mean between the cell and its neighbour. This is done for all cell walls and hence gives a locally anisotropic conductivity, i.e. for a given cell all cellwall conductivities are different.

- Calculate the length of the fracture zone crossings for each cell wall. Modify the cellwall conductivity with respect to the transmissivity of the fracture zones.

- Modify the conductivity for the top four layers. This is done as a condition; "if the cell wall conductivity is smaller than the prescribed conductivity for the cell layer, the prescribed value is used".

- Finally, modify conductivities with respect to unsaturated conditions. As this modification depends on the pressure, which is part of the calculation, it needs to be done during the iteration process.

Further details about the third point can be found in Svensson (1997).

3.5 BOUNDARY CONDITIONS

At the top boundary a net recharge, according to Figure 1-2, is specified above sea level. Below the Baltic Sea a hydrostatic pressure is prescribed, with respect to the local water depth, and the salinity is fixed to the salinity of the Baltic. The water level and salinity in the Baltic were given in Figure 1-2. When Äspö becomes an island in a freshwater lake, the pressure is prescribed below the lake, with respect to local water depth and freshwater density.

At the vertical and bottom boundaries zero flux conditions are used for all variables.

3.6 NUMERICAL TOOL AND OUTPUT PARAMETERS

The system of equations is solved by the general equation solver PHOENICS, Spalding (1981). PHOENICS is based on a finite-volume formulation of the basic equations and embodies a wide range of coordinate systems (cartesian, body-fitted, cylindrical, etc) and numerical techniques (higher order schemes, solvers, etc).

The basic output parameters from the model are pressure, salinity and Darcy velocities. It is however simple to generate additional output parameters like hydraulic head and density.

4 RESULTS

4.1 INTRODUCTION

The simulation produces more data that can be presented and discussed as we solve for thirteen variables in a high resolution grid and for a time period of 15 000 years. In the presentation of results we will first focus on the distribution of different water types at five selected times (7 000 BP, 6 000 BP, 3 000 BP, 0 BP and 5 AP), and after that we will discuss conditions below Äspö.

4.2 DISTRIBUTION OF WATER TYPES

The main water types at 7 000 years BP are shown in Figures 4-1 and 4-2. From Figure 1-2 it is clear that only two stages of the Baltic Sea, i.e. the Yoldia and Ancylus periods, have past at this time. However, one may of course also find water types set as initial conditions (Brine and Glacial meltwater) and Meteoric water (fresh recharge water). The Glacial meltwater fraction was found to be very small at 7 000 BP, which means that it can not dominate at later times either. The general impression from Figures 4-1 and 4-2 is that the Yoldia water fills the space above 1 000 metres depth except for a thin layer close to ground, where fresh Ancylus water resides.

At 6 000 years BP the Litorina period has started. The salinity of the Litorina water reaches a maximum of 1.4 %, which is the highest salinity during the 15 000 years considered. This heavy water replaces almost all other water types down to a depth of about 1 000 metres, where the even saltier water is found, as can be seen in Figures 4-3 and 4-4.

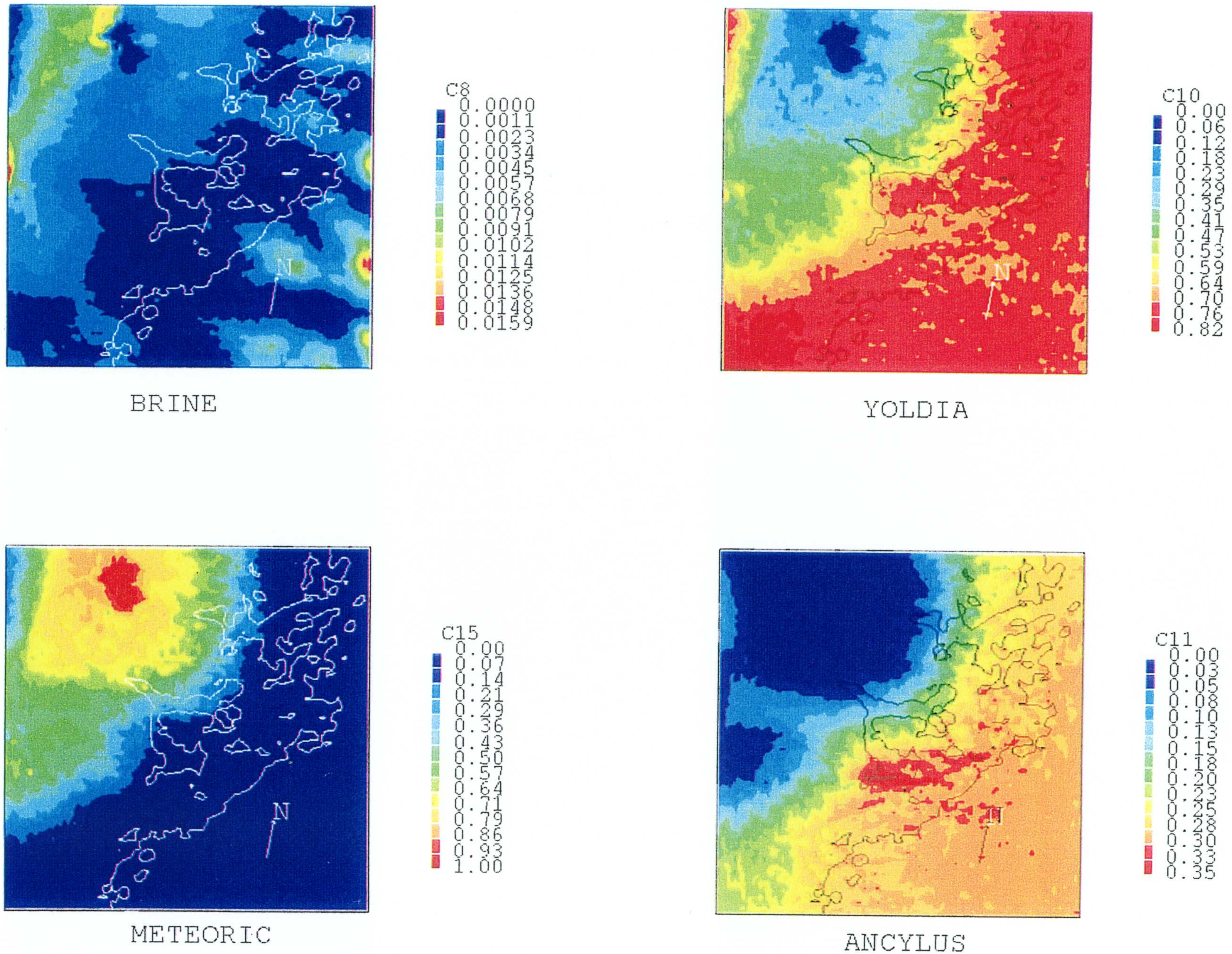

Figure 4-1. *Horizontal sections at a depth of 450 metres, showing the volume fractions of the dominant water types. Time: 7 000 years BP.*

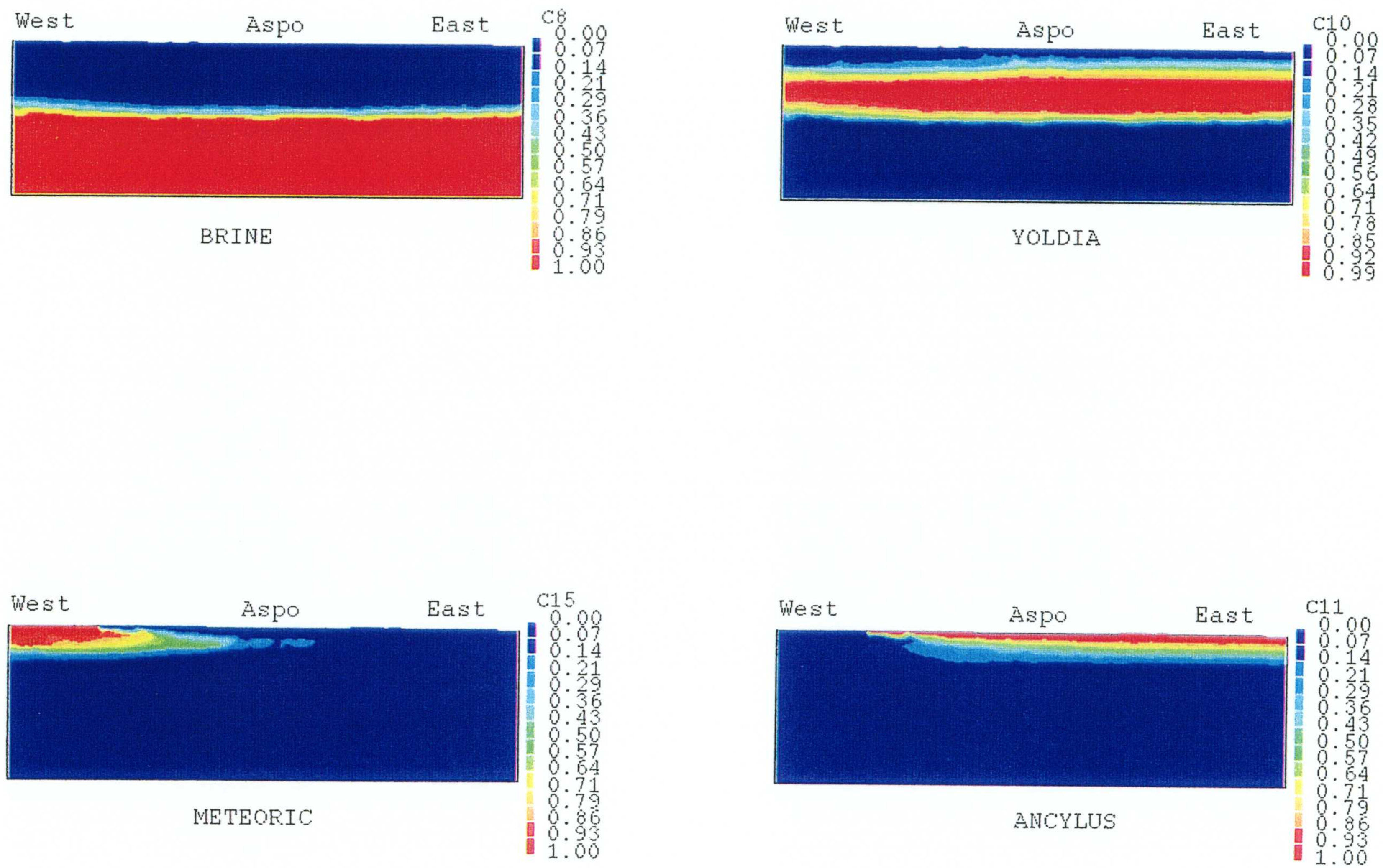

Figure 4-2. *Vertical east-west sections through the island of Äspö, showing the volume fractions of the dominant water types. Time: 7 000 years BP.*

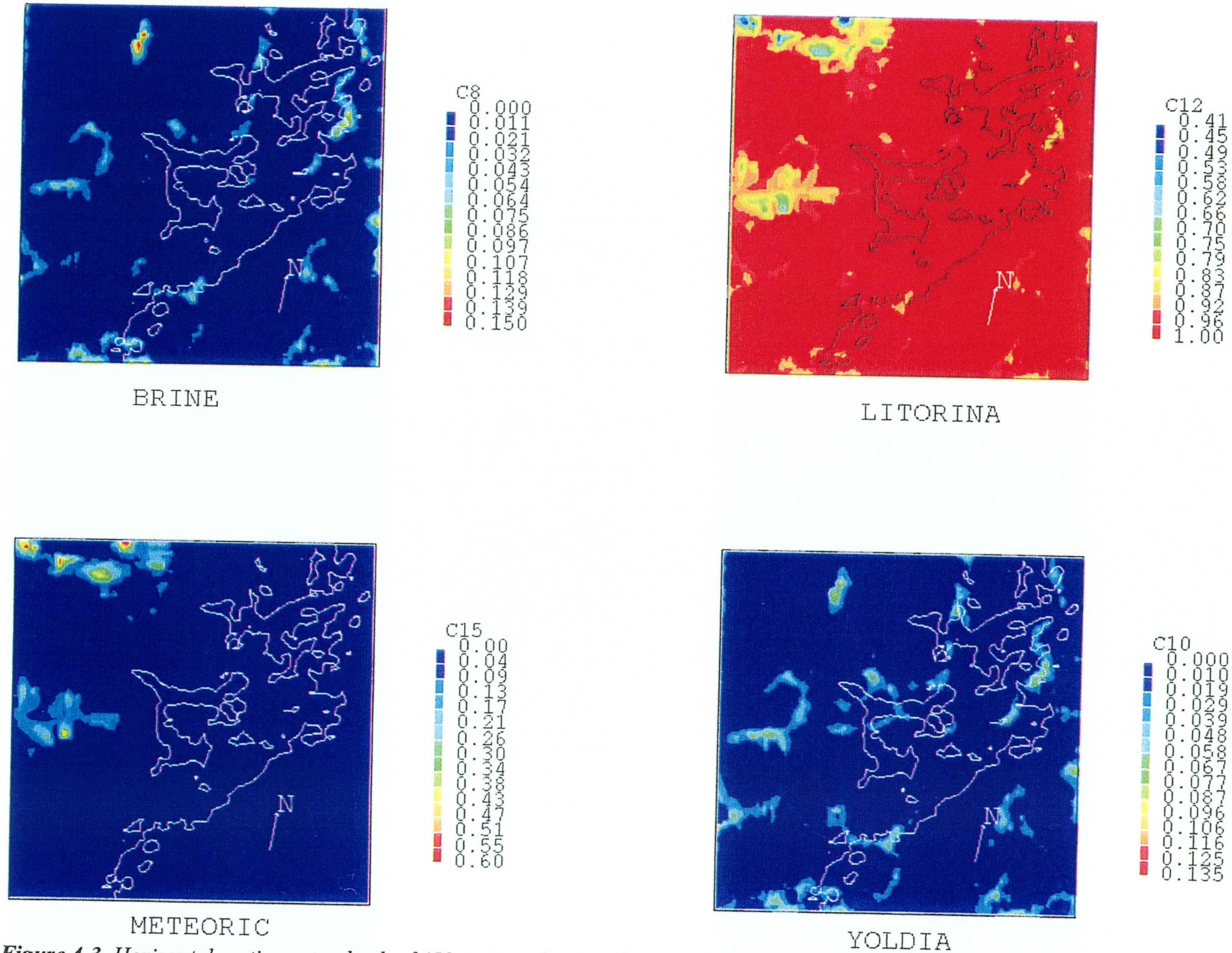

Figure 4-3. *Horizontal sections at a depth of 450 metres, showing the volume fractions of the dominant water types. Time: 6 000 years BP.*

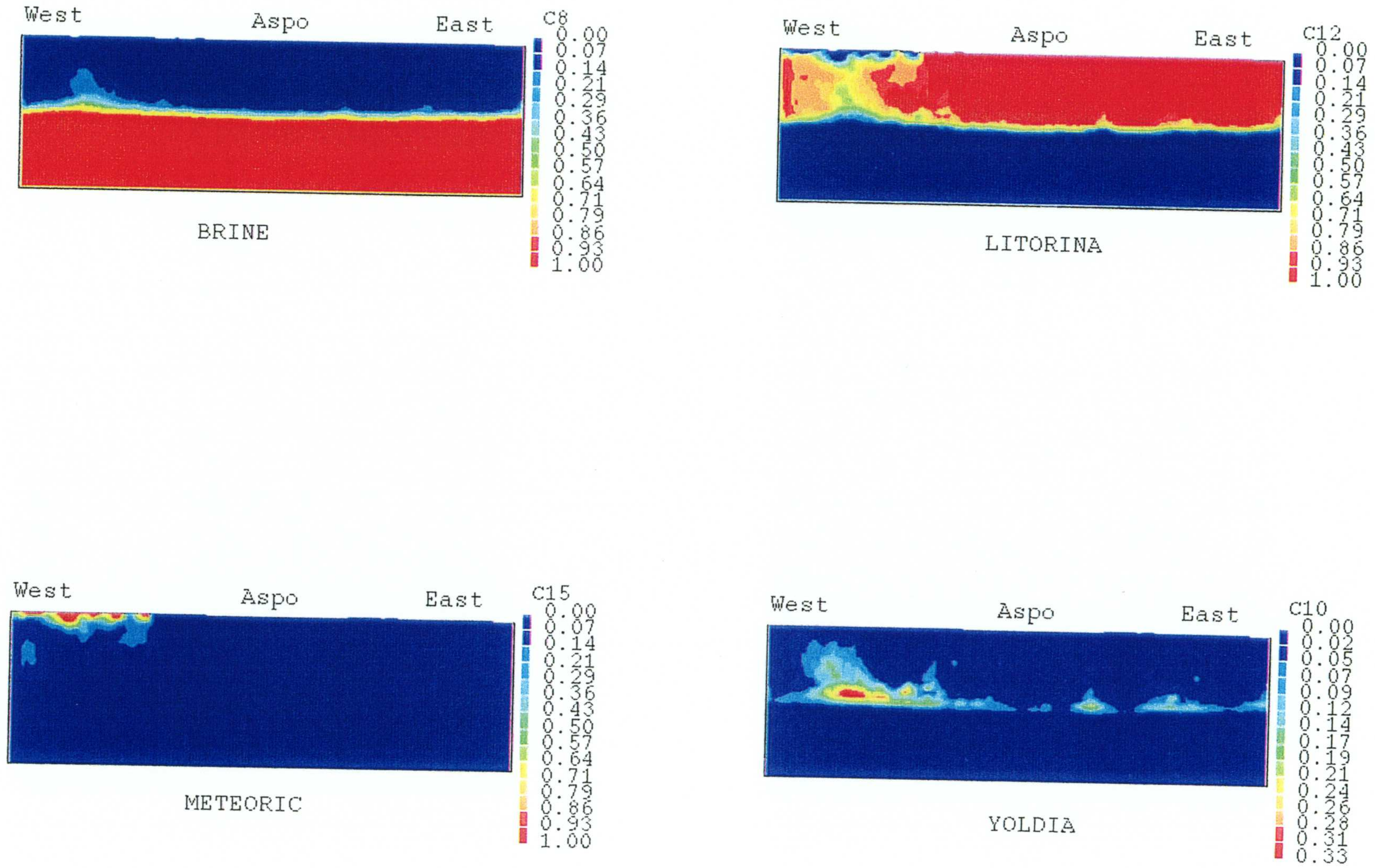

Figure 4-4. *Vertical east-west sections through the island of Äspö, showing the volume fractions of the dominant water types. Time: 6 000 years BP.*

Äspö became an island at about 4 000 years BP; the water level in the Baltic Sea was then about 10 metres above the present mean level. The next set of snapshots is from 3 000 years BP, which is in the Limnea period. The Baltic Sea had a salinity of 1.0 % at this time, which is somewhat smaller than the Litorina water. It is thus not surprising, see Figures 4-5 and 4-6, that the Limnea water floats on top of the Litorina water. Another thing to note in the figures is that the freshwater lens in the high areas west and north of Äspö is now well established.

The present conditions, are shown in Figures 4-7 and 4-8. According to these figures the water below Äspö, at a depth of 450 metres, is composed of Meteoric and Brine water; a result that certainly needs to be discussed and analysed further. The Baltic water around Äspö can not penetrate into the ground as Äspö and the sea around Äspö is a discharge area. The discharge water origins from the Laxemar area and brings up the Brine water due to the circulation in the freshwater lens.

Finally the conditions at 5 000 AP are presented, see Figures 4-9 and 4-10. Now the water level in the Baltic is 6 metres below present level and the waters around Äspö are freshwater lakes. The main characteristic feature at this time is the large fresh water lens that brings up some Brine at the coastline. The coastline is however now close to the east model boundary and the distributions can be expected to be influenced by the zero flux condition used at this vertical boundary.

4.3 CONDITIONS BELOW ÄSPÖ

The evolution of the water composition at a point 450 metres below Äspö can be studied in Figure 4-11. The history is essentially as described with the snapshots above and we can see that the present water is composed of Brine and Meteoric water. However, if we go back 1 000 years the dominant water type was Baltic.

The vertical distribution of water components below Äspö, at present time, is shown in Figure 4-12. At 450 metres depth the Brine and Meteoric water types dominate, but at a depth of about 1 000 metres there is also a significant fraction of Litorina water. Also small fractions of Limnea and Baltic waters are found at this depth.

The transport time from 300 → 700 metres depth is illustrated in Figures 4-13 and 4-14. Particles were released along a vertical line at a central position below Äspö and tracked for 500 years. No dispersion effects were considered. The pore velocity, which is used for the particle transport, was related to the Darcy velocity

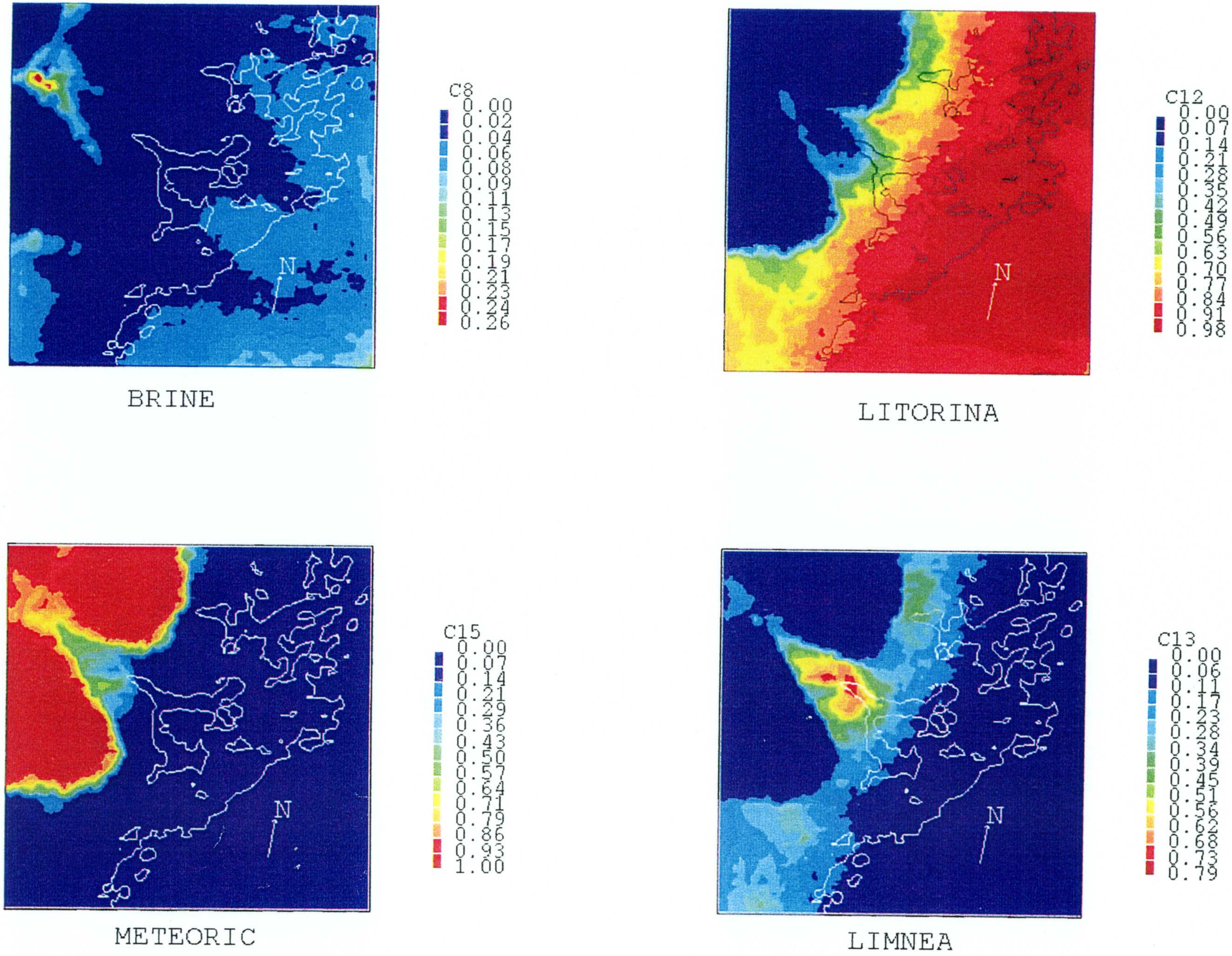

Figure 4-5. *Horizontal sections at a depth of 450 metres, showing the volume fractions of the dominant water types. Time: 3 000 years BP.*

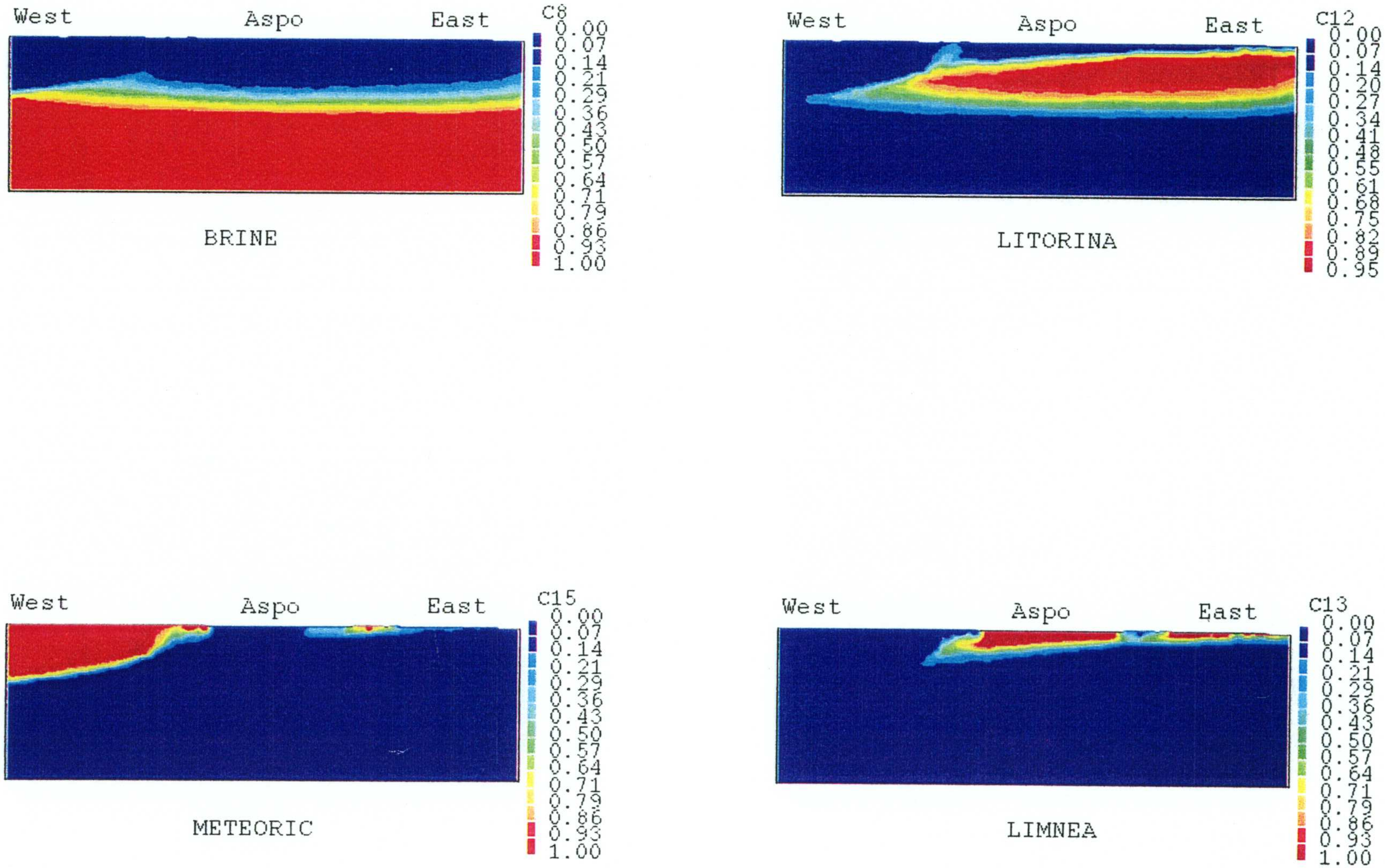

Figure 4-6. *Vertical east-west sections through the island of Äspö, showing the volume fractions of the dominant water types. Time: 3 000 years BP.*

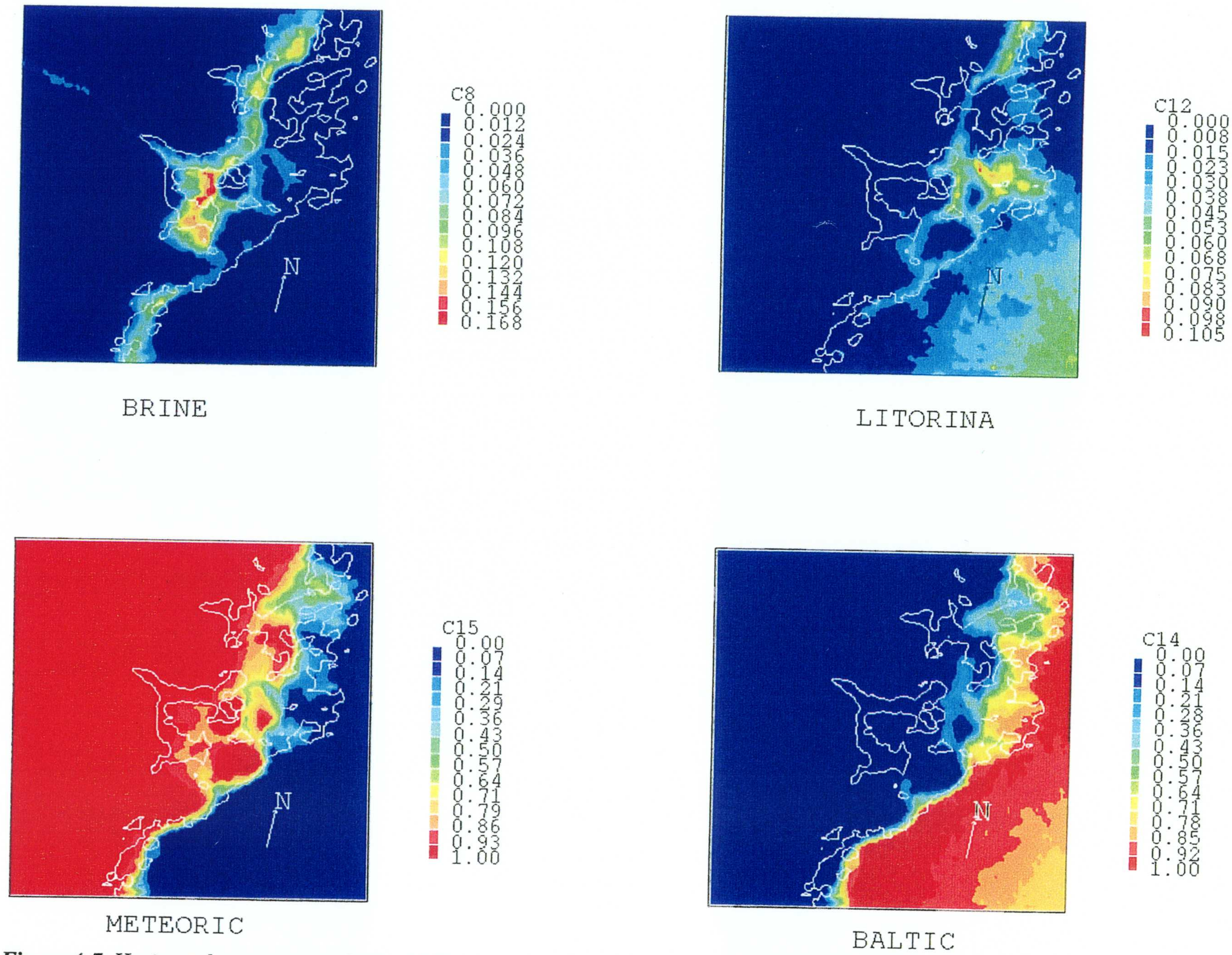

Figure 4-7. *Horizontal sections at a depth of 450 metres, showing the volume fractions of the dominant water types. Time: 0 year BP.*

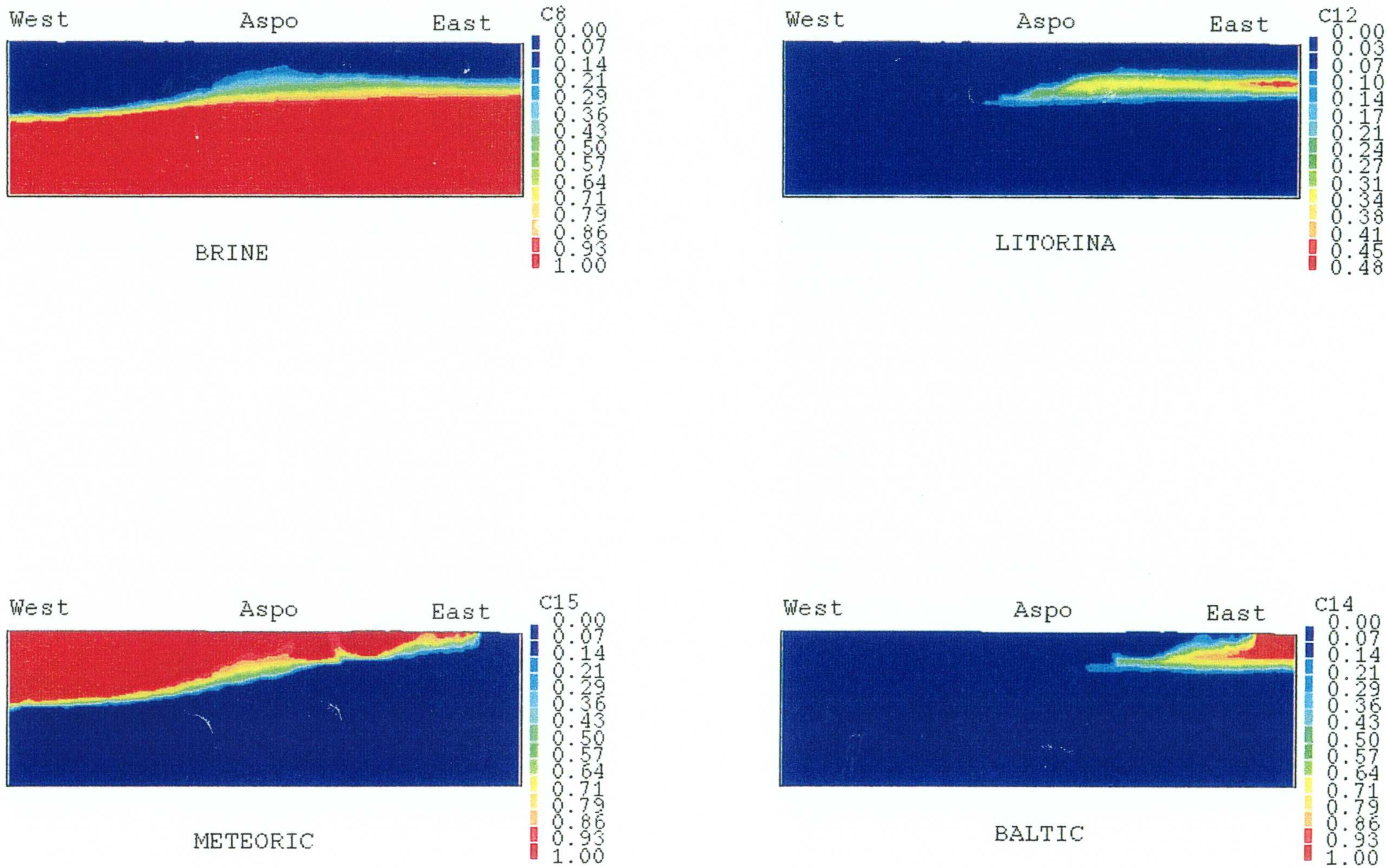

Figure 4-8. *Vertical east-west sections through the island of Äspö, showing the volume fractions of the dominant water types. Time: 0 year BP.*

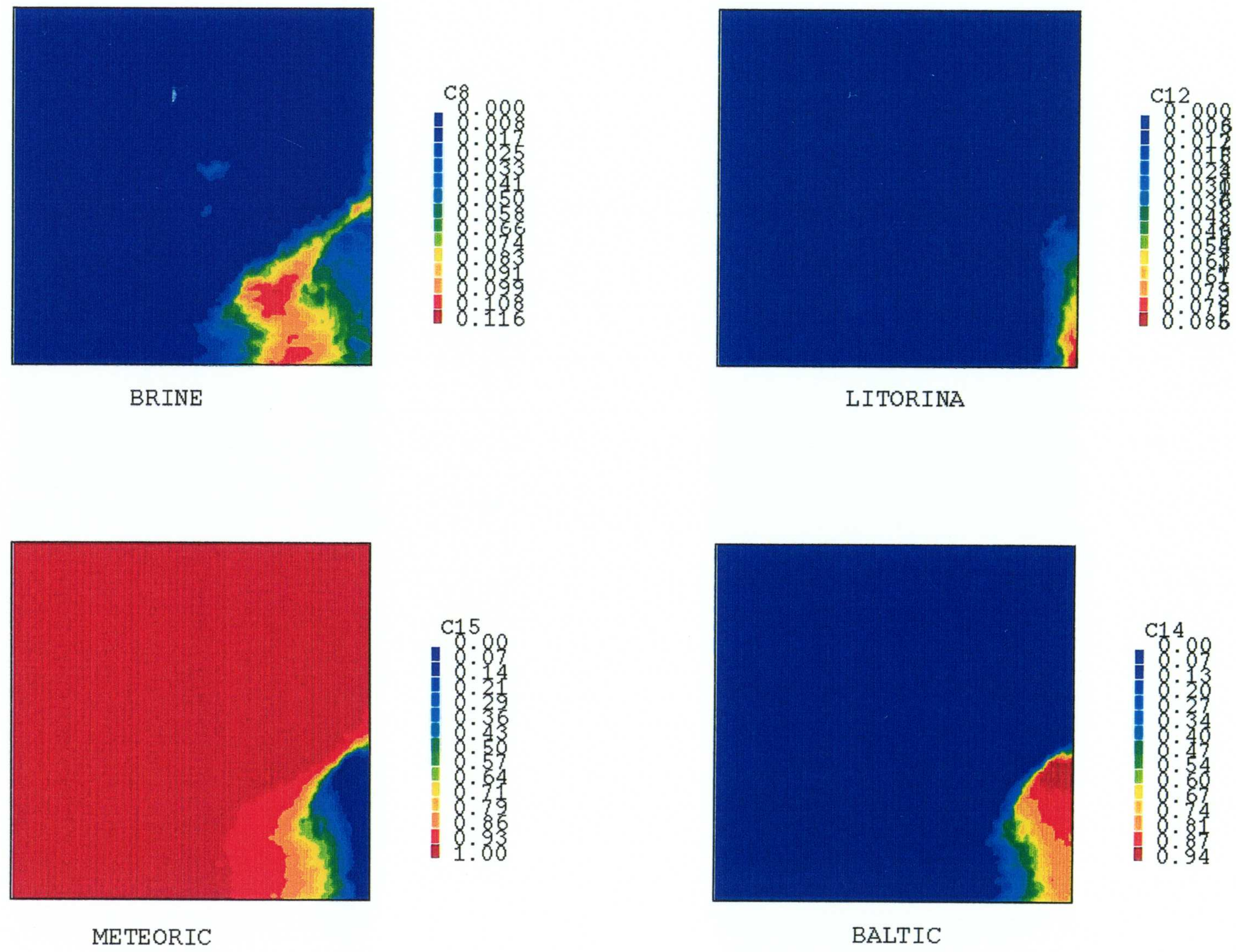

Figure 4-9. *Horizontal sections at a depth of 450 metres, showing the volume fractions of the dominant water types.* Time: 5 000 years AP.

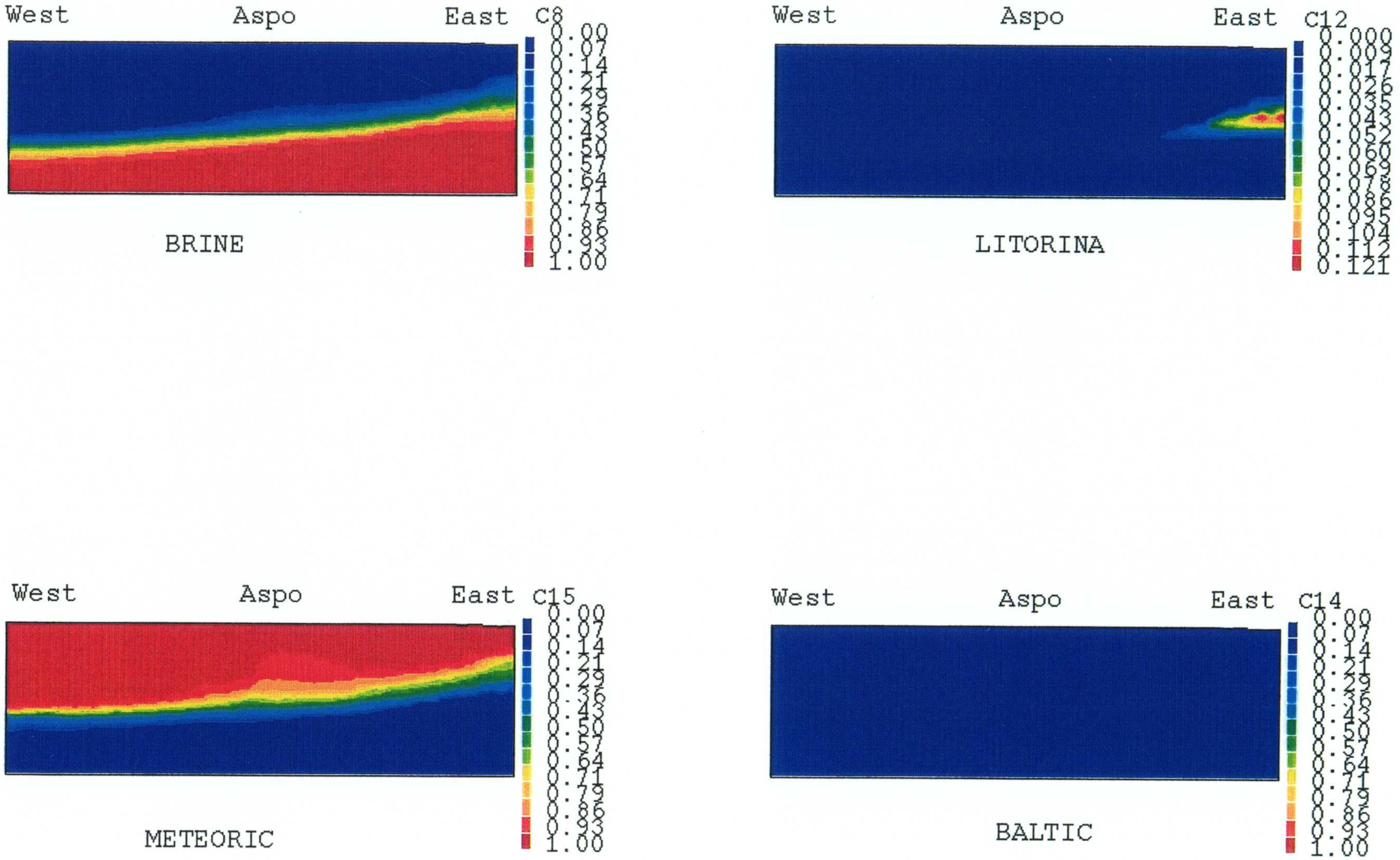

Figure 4-10. *Vertical east-west sections through the island of Äspö, showing the volume fractions of the dominant water types. Time: 5 000 years AP.*

through a kinematic porosity, n_e. In Rhén et al (1997) a relation between the hydraulic conductivity (K) and n_e is suggested:

$$n_e = 34.87K^{0.753} \quad (4\text{-}1)$$

This equation was used with the constraint that $n_e \leq 0.05$.

The simulations reflect the strong influence of the density stratification. At 7 000 years BP the typical pore-velocity is of the 10^{-8} m/s, which gives a displacement of 0.3 metres/year. It is thus not surprising that no particles reach ground level in the 500 years the particles were tracked. At 3 000 years BP most particles reach ground level in 500 years; the typical transport time is around 400 years. For present conditions (0 years BP) it is clearly seen that we have stagnant condition below 500 metres while particles released above this level will reach ground level in about 20 years. For 5 000 years AP we find even shorter transport times, which can be expected as Äspö is now a discharge area.

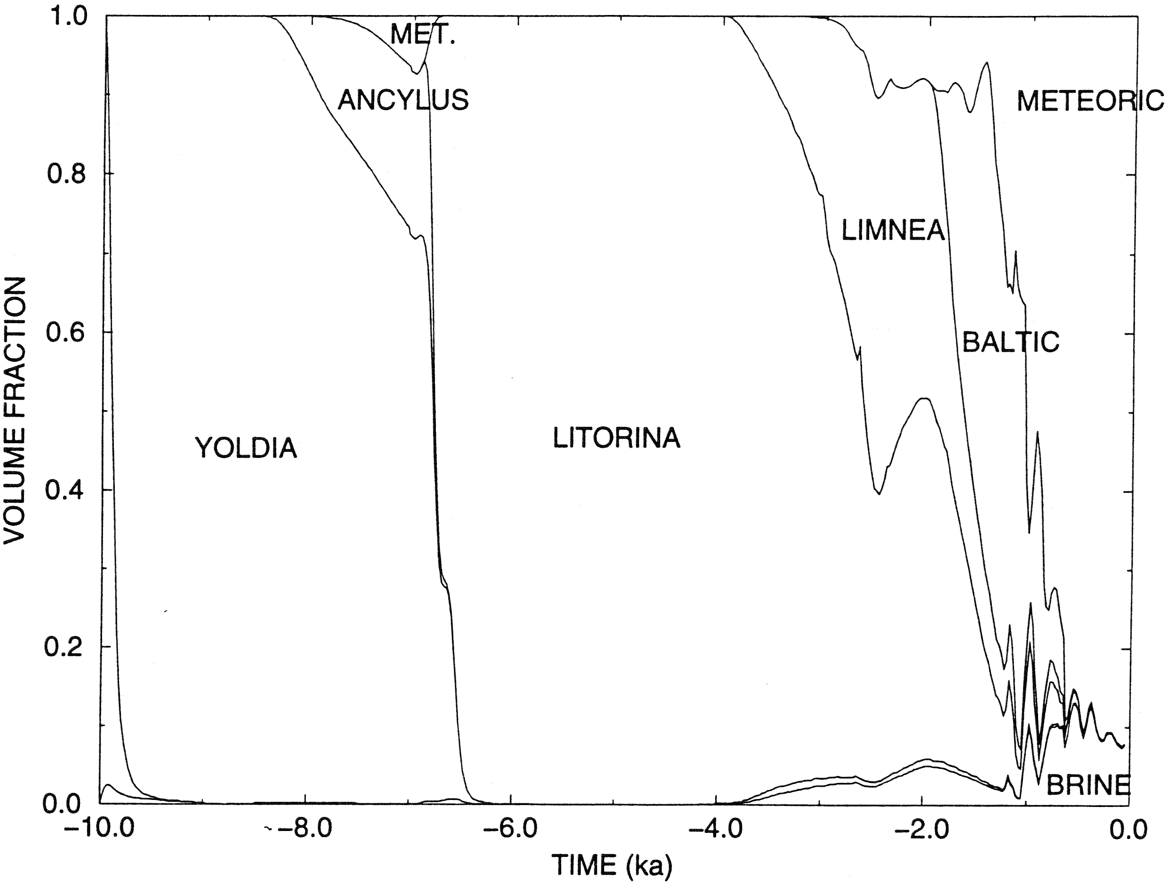

Figure 4-11. *The evolution of the ground water composition at a point 450 metres below Äspö.*

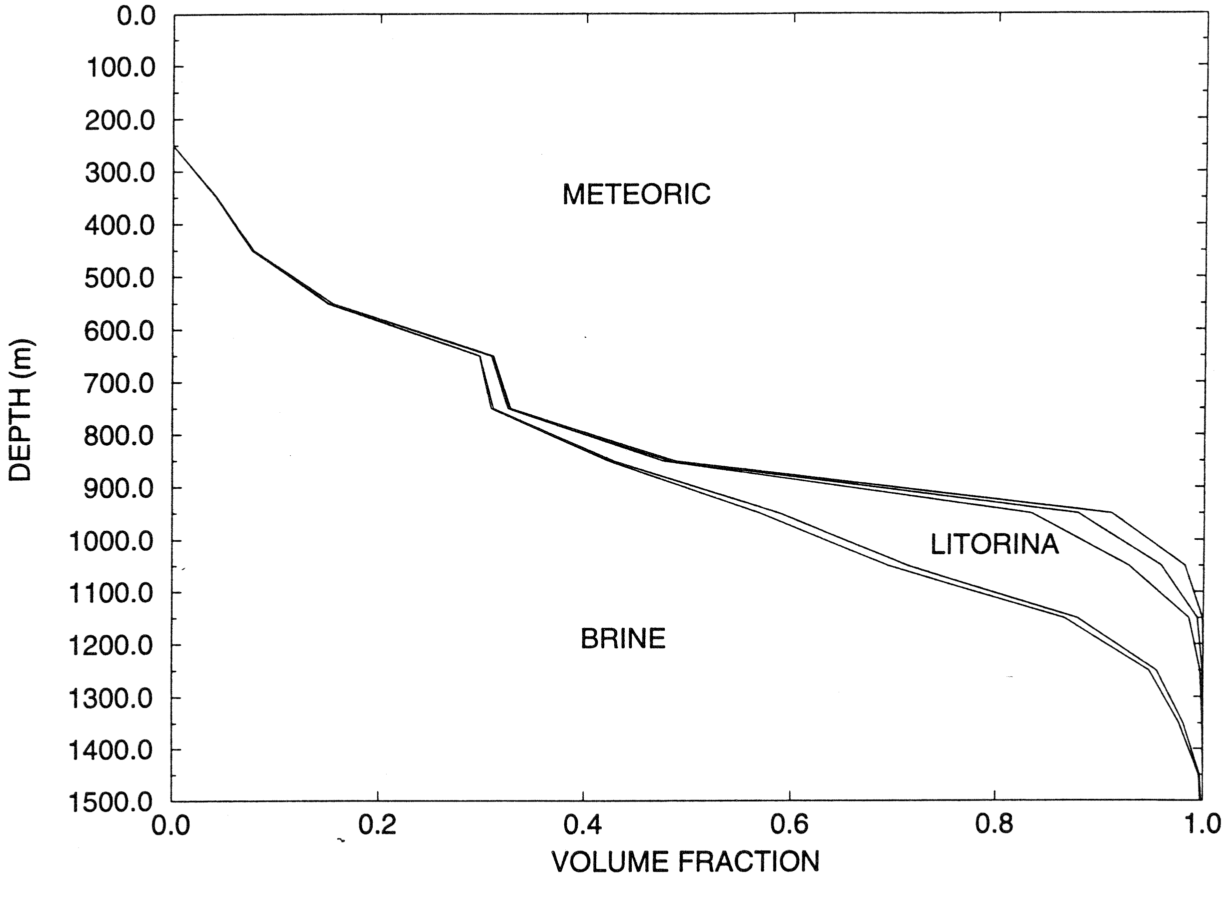

Figure 4-12. *Ground water composition versus depth at Äspö for present time.*

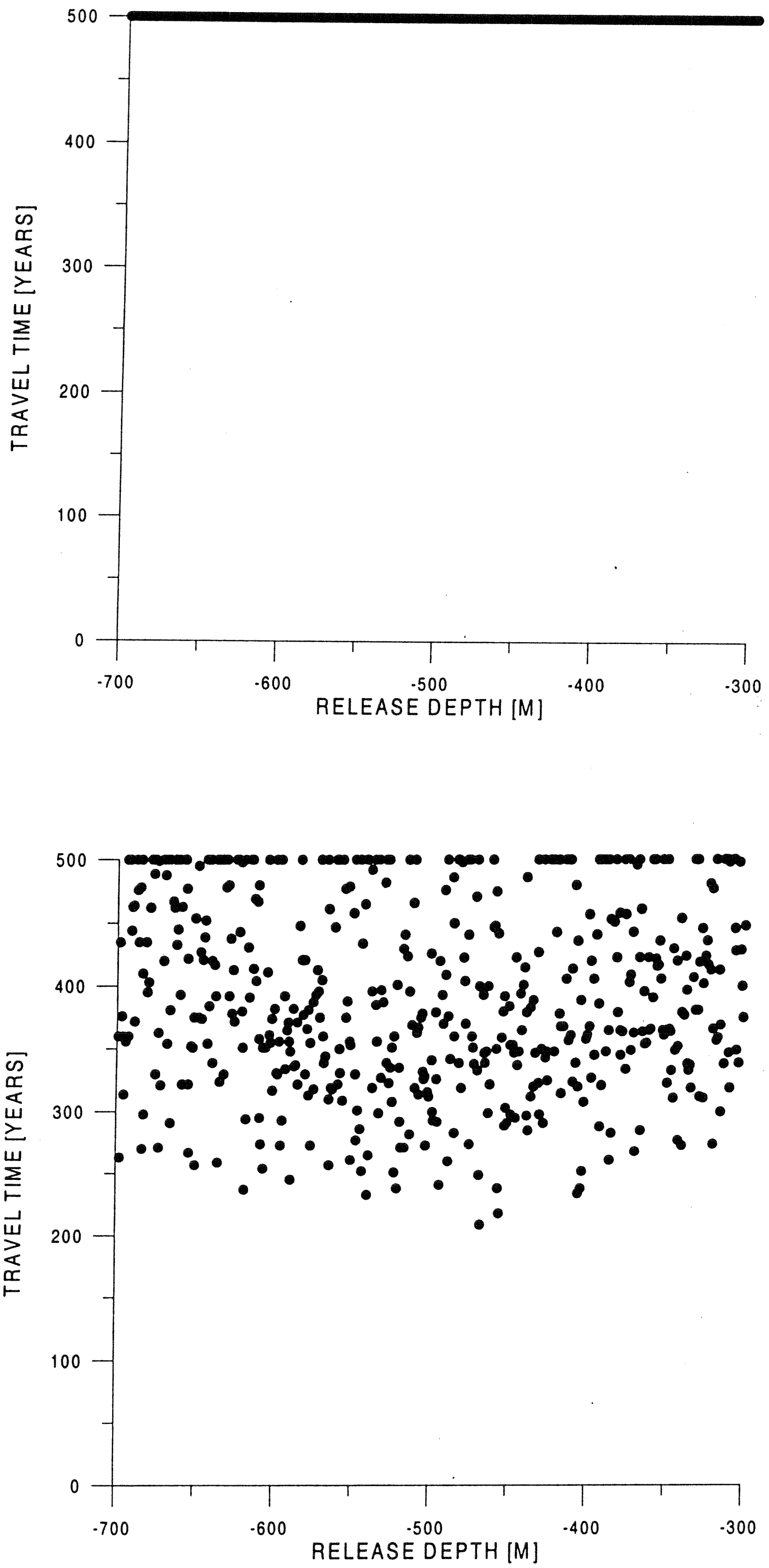

Figure 4-13. *Travel time from the depth interval -700 → -300 metres 7 000 years BP (top) and 3 000 years BP. 500 particles were released and tracked for a maximum time of 500 years.*

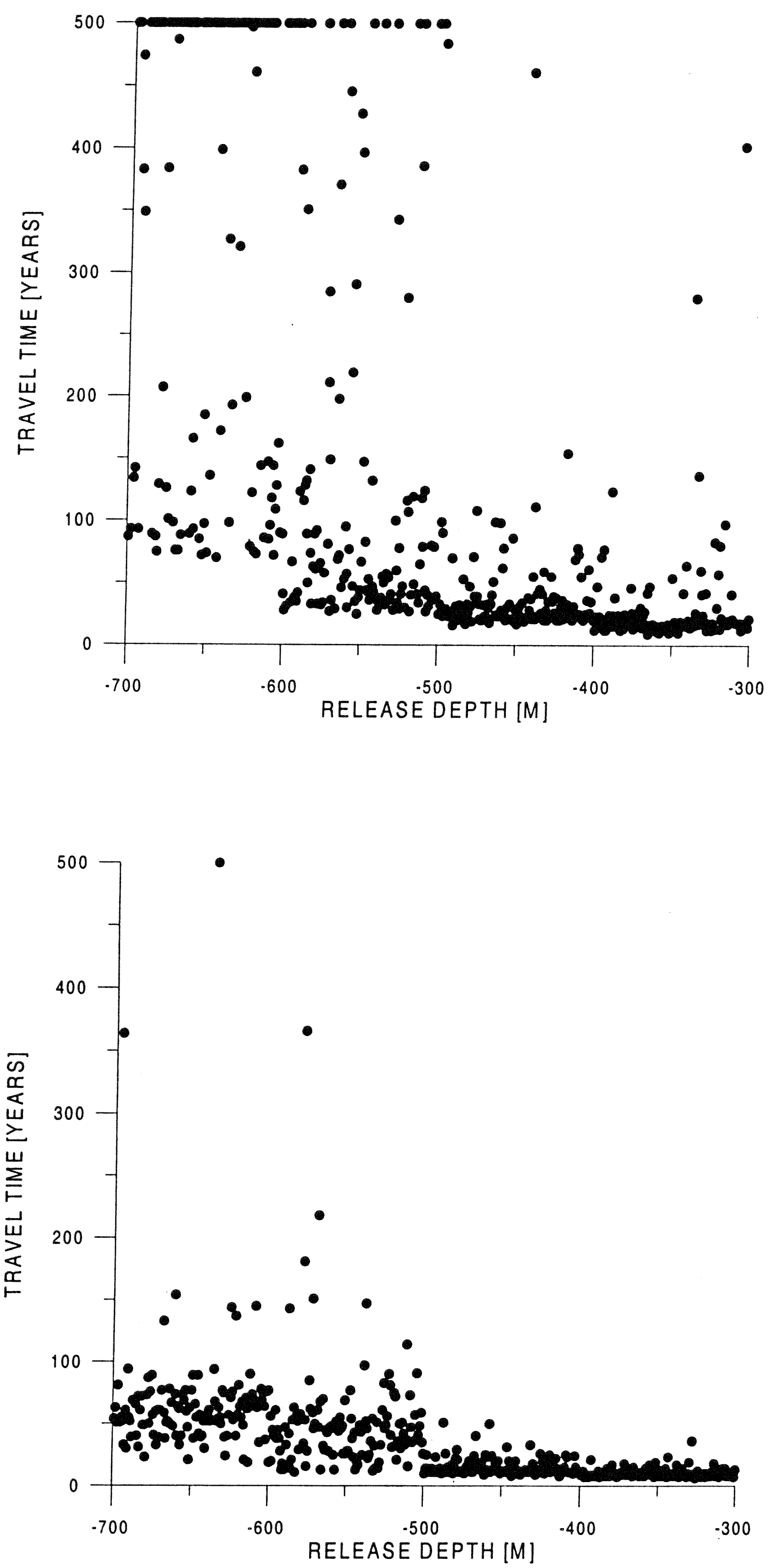

Figure 4-14. *Travel time from the depth interval -700 → -300 metres 0 years BP (top) and 5 000 years AP. 500 particles were released and tracked for a maximum time of 500 years.*

5 DISCUSSION AND CONCLUSIONS

The results presented demonstrate that it is possible to handle the computationally heavy problem addressed (long-term transient, thirteen variables, high resolution body-fitted grid, etc). It was the main objective of the study to evaluate if simulations like the one carried out are feasible. All results look plausible, but it should be remembered that several assumptions were made in order to simplify the problem. We can now list some of these as suggestions for future investigations:

- Upper boundary conditions. It is the water level and salinity of the Baltic Sea and the freshwater recharge on land that are the main governing effects in the problem. Refined knowledge about these boundary conditions is essential.

- Regional influence. Does a larger scale regional flow influence the conditions below Äspö? If so, how should it be accounted for?

- Double porosity effects. It can be expected that water is stored in cavities and other stagnant parts of the rock. This effect is presently not accounted for in the simulation model.

- Tracking a fluid component with an advection/diffusion equation, as done in this study, is known to cause problems with numerical diffusion. Higher order numerical schemes should be tried in order to evaluate the effect.

- Mixing, dispersion and chemical reactions between different end-members are known to take place. These effects also need to be considered in the simulation model.

Apparently, the model can, and need, to be improved before we can make quantitative comparisons between measured and calculated water composition below the island of Äspö. This first step, the feasibility, is however regarded as successful and should encourage to further development.

6 REFERENCES

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APPENDIX A

Some additional results requested by the performance and safety assessment project (SR97).

Some additional results requested by the performance and safety assessment project (SR97)

Background

The results presented in this report have been found to be of interest for safety assessment studies. As a response to this interest some additional simulations were carried out. The objective of this Appendix is to present these.

Results

The first additional information concerns Figures 4-13 and 4-14, where the transport time from 300 $\rightarrow$ 700 metres depth below Äspö is given. For the four times (7 000 BP, 3 000 BP, 0 BP and 5 000AP) the Darcy flow in the start positions has been requested. This information is given in Table A1. As can be seen the flow is extremely small for 7 000 BP, which is also reflected in Figure 4-13. The median travel time to reach ground level for the four times was also estimated; this information is found in Table A2.

The almost stagnant conditions at 7 000 years BP are also illustrated in Figure A1, where particle positions after 500 years of integration are shown. 500 particles were released at 450 metres depth in a rectangular area (200 x 200 m^2) centred around Äspö HRL. When the flow field from 7 000 BP is used the particles are hardly moved at all in 500 years. The flow field at 3 000 BP moves the particles towards the Laxemar area. The reason for this is that the particles are now east of the salt/freshwater interface. At 0 BP and 5 000 AP the particles are in the discharge area and hence reach ground level much faster.

Table A1. Darcy flow in the startpositions of the particles illustrated in Figures 4-13 and 4-14.

Time	Äspö coordinates (m)			Velocities (m/s)			
years	east	north	vertical	east	north	up	magnitude
7 000BP	2050	7350	-350	$0.44x10^{-12}$	$-0.69x10^{-12}$	$-0.18x10^{-12}$	$0.84x10^{-12}$
	2050	7350	-450	$-0.15x10^{-12}$	$0.23x10^{-12}$	$-0.13x10^{-12}$	$0.30x10^{-12}$
	2050	7350	-550	$-0.35x10^{-12}$	$0.21x10^{-12}$	$-0.12x10^{-12}$	$0.43x10^{-12}$
	2050	7350	-650	$-0.49x10^{-12}$	$0.72x10^{-12}$	$-0.18x10^{-12}$	$0.88x10^{-12}$
3 000BP	2050	7350	-350	$-0.37x10^{-10}$	$0.14x10^{-10}$	$0.45x10^{-12}$	$0.40x10^{-10}$
	2050	7350	-450	$-0.12x10^{-10}$	$0.13x10^{-10}$	$-0.23x10^{-12}$	$0.17x10^{-10}$
	2050	7350	-550	$-0.20x10^{-10}$	$0.27x10^{-11}$	$0.34x10^{-11}$	$0.20x10^{-10}$
	2050	7350	-650	$-0.19x10^{-10}$	$0.56x10^{-11}$	$0.41x10^{-11}$	$0.20x10^{-10}$
0BP	2050	7350	-350	$0.28x10^{-9}$	$-0.17x10^{-9}$	$-0.33x10^{-10}$	$0.32x10^{-9}$
	2050	7350	-450	$0.46x10^{-10}$	$-0.45x10^{-10}$	$0.69x10^{-11}$	$0.65x10^{-10}$
	2050	7350	-550	$0.39x10^{-10}$	$-0.65x10^{-11}$	$0.31x10^{-11}$	$0.39x10^{-10}$
	2050	7350	-650	$0.17x10^{-10}$	$-0.11x10^{-10}$	$0.42x10^{-12}$	$0.21x10^{-10}$
5 000AP	2050	7350	-350	$0.61x10^{-9}$	$-0.23x10^{-9}$	$-0.28x10^{-9}$	$0.71x10^{-9}$
	2050	7350	-450	$0.14x10^{-9}$	$-0.11x10^{-9}$	$-0.15x10^{-10}$	$0.18x10^{-9}$
	2050	7350	-550	$0.18x10^{-9}$	$0.41x10^{-11}$	$-0.69x10^{-11}$	$0.18x10^{-9}$
	2050	7350	-650	$0.19x10^{-9}$	$0.10x10^{-9}$	$0.29x10^{-10}$	$0.21x10^{-9}$

Table A2. Median travel time to ground level for particles illustrated in Figures 4-13 and 4-14.

Time (years)	Median travel time (years)
7 000BP	>10 000
3 000BP	402
0BP	50
5 000AP	26

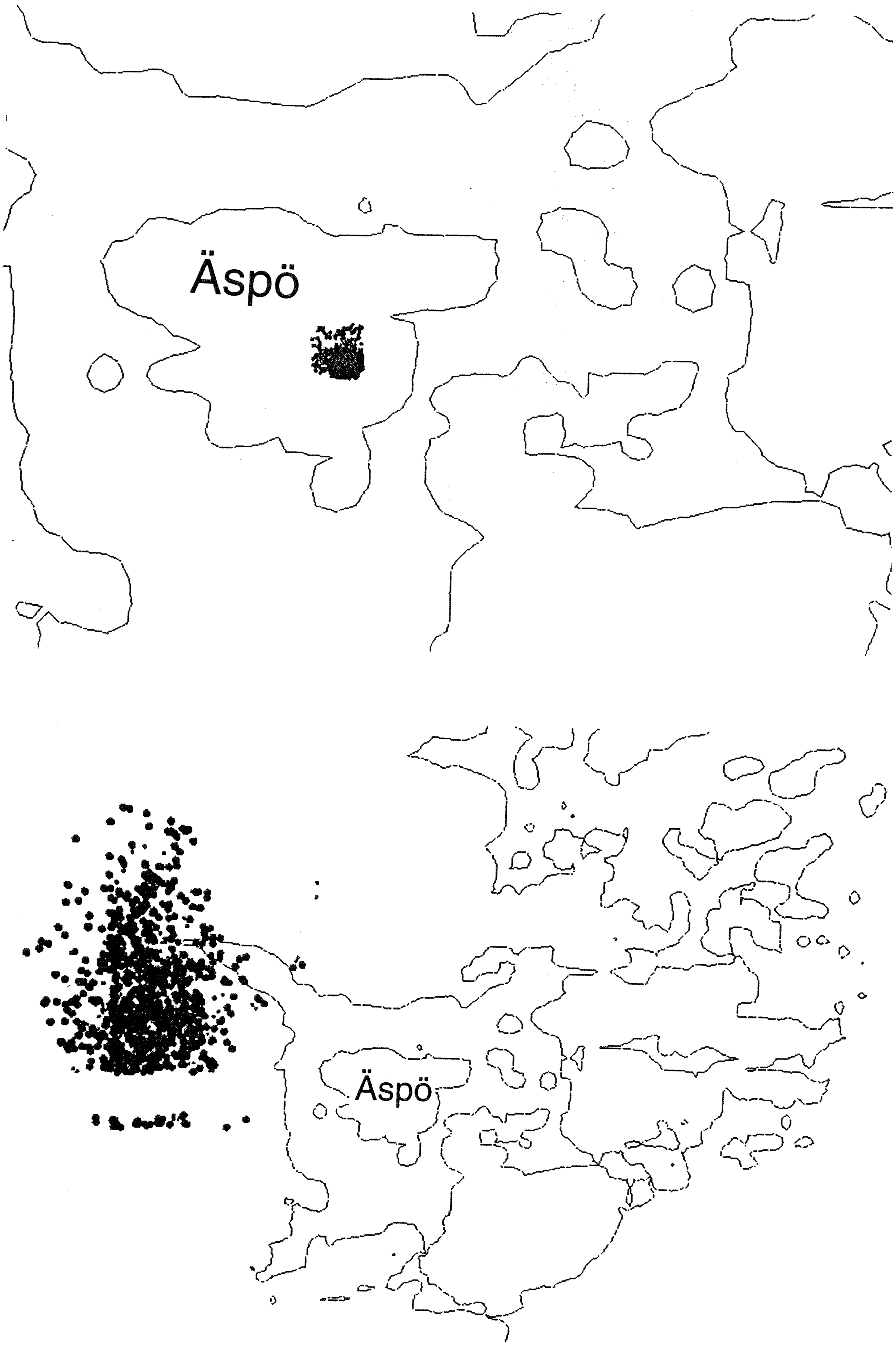

Figure A1. *Particle positions after 500 years of integration. Startpositions at 450 metres depth in a rectangle centred around Äspö HRL. Big particles are close to surface, smaller ones at deeper levels. Flow field from 7 000BP (top) and 3 000BP.*

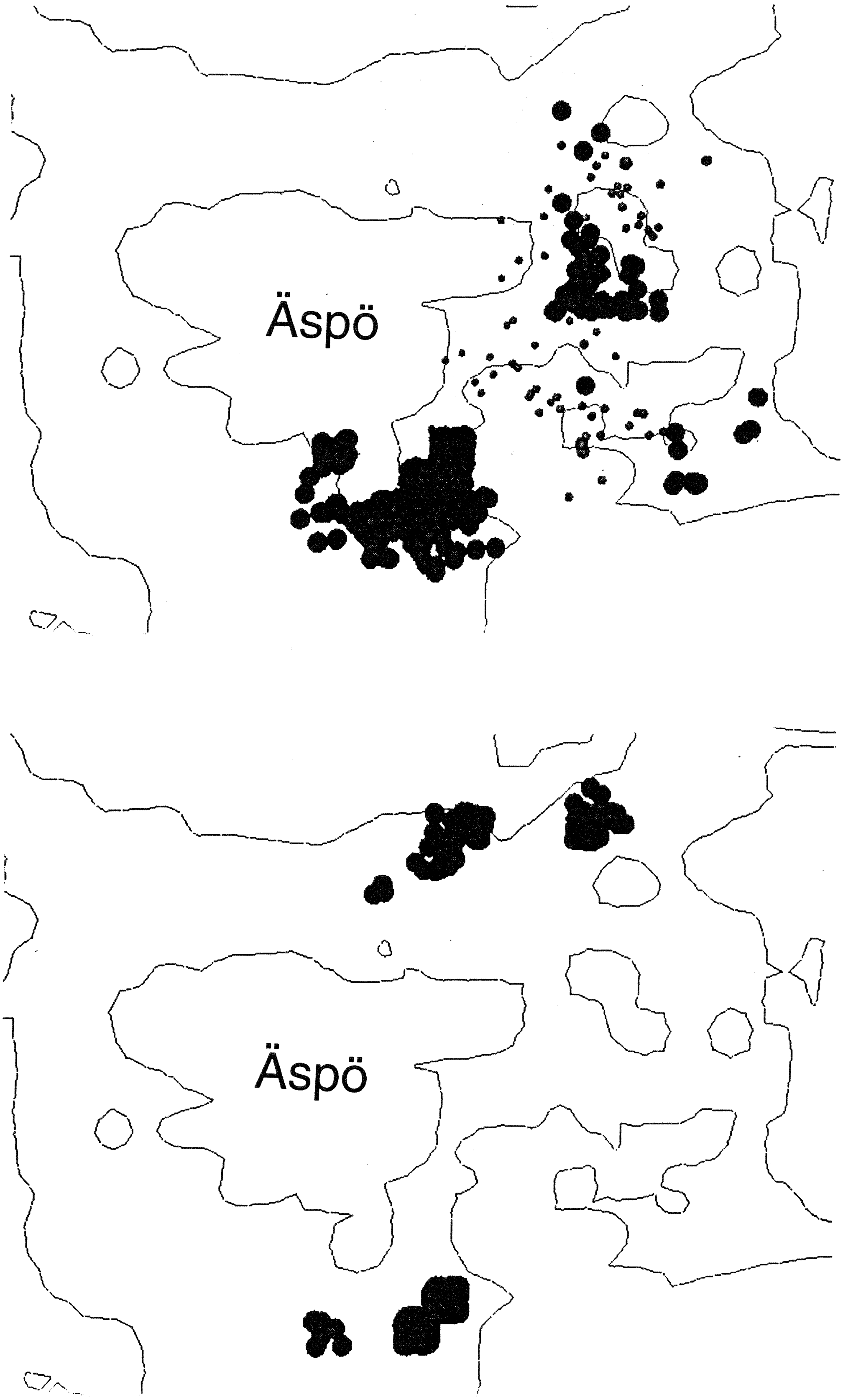

Figure A1, *Cont. Flow field from 0BP (top) and 5 000AP.*

APPENDIX B

DOCUMENTATION

SKB-ÄSPÖ HARD ROCK LABORATORY

Documentation of numerical simulation by Urban Svensson (US) 1998-04-14

OBJECT

SKB purchase order no: 82030-97-129
Title of SKB purchase order: SR97 – Regional geohydrologisk analys av effekter av strandförskjutning.
Author of report: US — Company: CFE AB
Operator of computer and software: US — Company: CFE AB

COMPUTER

Name and version: Silicon Graphics, O2/R10 000.

SOFTWARE

Operative system: IRIX 6.3
Code name: PHOENICS 2.1 — Main manual: On line
Program language: FORTRAN
Compiler: F77 for IRIX 6.3
Postprocessor name: PHOTON — Manual:
Subroutine: — Report:
Subroutine: — Report:
Subroutine: — Report:

CODE VERIFICATION

Distributor: Not compiled in a single report.
Report/article:
Report/article:
Other verification
Report/article: See Svensson (1995) and (1997), as referenced in this report.
Report/article:

INPUT DATA

Ref: Rhén et al (1997), see reference list.
Ref: Westman (1997)
Ref: Påsse (1996)
Ref:

Data file name:	Data of issue:	Stored at:
Data file name:	Data of issue:	Stored at:
Data file name:	Data of issue:	Stored at:

RESULTS

Report/article: All given in this report.
Report/article:

Data file name:	Stored at:
Data file name:	Stored at:

CONDENSED DESCRIPTION OF GROUNDWATER FLOW MODEL.

A numerical simulation of the origin and composition of the groundwater below Äspö Stochastic continuum model	
Scope: Origin and composition of groundwater at Äspö	
Process description Conservation of mass, volume and momentum (Darcy's law)	
CONCEPTS	**DATA**
Geometric framework and parameters	
Domain divided into computational cells to which conservation laws are applied. Subdomains consist of deterministic fracture zones and rock volumes between the fracture zones.	Domain size: 10 x 10 x 3 km^3 Computational grid: 360 000 cells
Material properties	
Hydraulic conductivities (K). Density varies with salinity. Transmissivity for fracture zones (T).	Data from Rhén et al (1997).
Spatial assignment method	
Stochastic conductivity for the rock mass outside the deterministic fracture zones with no correlation between cells. Deterministic fracture zone transmissivities. K modified if cell is intersected by a fracture zone.	Data from Rhén et al (1997).
Boundary conditions	
Prescribed pressure and salinity below the Baltic and prescribed recharge on land. Zero flux condition on vertical and bottom boundaries.	Data from Westman (1997) and Påsse (1996).
Numerical tool PHOENICS	
Output parameters Flux, pressure and salinity.	