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Effects of variations in hydraulic conductivity and flow conditions on groundwater flow and solute transport in peatlands

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This report concerns a study which was conducted for SKB. The conclusions and viewpoints presented in the report are those of the author and do not necessarily coincide with those of the client.

A pdf version of this document can be downloaded from www.skb.se.

Abstract

In this report it is examined to what extent the variation in hydraulic conductivity within a peatland and adjoining sediments would affect the flow patterns within it under some certain hydraulic-head gradients and other certain border conditions. The first part of the report contains a short review of organic and mineral-soil sediment types and characteristics and what we know about present peatlands and underlying sediments in the SKB investigation areas today. In the next part, a 2-dimensional model is used to simulate flows and transports in different settings of a peatland, with the objective of studying the effects of some particular factors:

1. The magnitude of the hydraulic conductivity of the peat and of underlying layers.
2. Presence and positions of cracks in underlying clay layers.
3. Anisotropy and heterogeneity in peat hydraulic conductivity.
4. The size of the water recharge at the peatland surface.
5. The seasonal variation of the water recharge.

The modelling results show that the importance of flow direction decreases with decreasing hydraulic conductivity in the peatland. This occurs as the convective flux is slowed down and the transport is taken over by the diffusive flux. Because the lowest hydraulic conductivity layer to large extent determines the size of the flow, presence of a low-conductivity layer, such as a layer of clay, is an important factor. Presence of cracks in such tight layers can increase the transport of solutes into the peat. The highest inflow rates are reached when such cracks occur in discharge areas with strong upward flow. On the other hand, a conservative solute can spread efficiently if there is a crack in low-flow locations.

The effect of anisotropy is found to be small, partly because the horizontal gradients become smaller as distances are larger. The effect of layers with high or low permeability varies depending on the location and the prevailing gradients. One tight layer has a strong effect on the flow pattern (in the same way as a clay layer), whereas a second tight layer influences less. Presence of a highly permeable horizontal layer increased the lateral flow but how the solute concentrations are enhanced by this depends on where the solute source is located.

The border conditions that determine the directions and sizes of fluxes are crucial for the resulting distributions. High flow rates, created by steep hydraulic-head gradients and permeable soils, generate clear differences between areas of inflow and outflow. When the flow rates are smaller, the importance of diffusion processes increases and the differences between areas of inflow and outflow get smaller.

A change in the size of the recharge (precipitation-evapotranspiration) can change the hydraulic-head pattern and flow paths, such that the distribution of solutes gets altered substantially. This has also the implication that seasonal shifts in the recharge may cause a seasonal variation in the distribution of a soluble compound. The same effect could occur when shifts in climate take place. As most peatlands are expected to develop from fen-types to bog-types, the expected final flow pattern may seem obvious and perhaps irreversible. However, temporal variations in recharge may create alternating periods of inflow and outflow from the underlying aquifer, and the relationships between time and rates in each direction determine the resulting distribution of a solute.

Sammanfattning

Svenska torvmarker har i regel utvecklats genom olika stadier med skiftande vattentillförsel, näringstillgång och klimat, resulterande i varierande våtmarksbiotoper och följaktligen varierande torvtyper. Årtusendens utveckling genom sådana olika stadier har lett till att dagens torvmarker kan innehålla lager av torv med mycket varierande egenskaper. En av dessa egenskaper som anses särskilt viktig för transport av ämnen med grundvattnet är markens genomsläpplighet, eller den hydrauliska konduktiviteten.

Som en del av utvecklingsarbetet för SKB:s säkerhetsanalys av ett djupförvar har det i denna studie undersökts i vilken utsträckning variationen av hydraulisk konduktivitet i en torvmark och i underliggande sediment kan påverka flödesmönstren i dess grundvatten. Första delen av denna rapport utgörs av en genomgång av olika typer av organiska och oorganiska sediment samt deras egenskaper och vad vi vet om lagerföljder hos nuvarande torvmarker i SKB:s undersökningsområden. I andra delen av detta arbete används en tvådimensionell hydraulisk flödesmodell för att simulera flöden och ämnestransporter hos torvmarker med några olika förutsättningar. Studiens syfte var först och främst att studera effekterna av följande faktorer:

1. Den hydrauliska konduktivitetens storlek i torvmarken och i underliggande lager.
2. Förekomst och läge av sprickor eller försvagningar i underliggande lerlager.
3. Anisotropi och heterogenitet i torvens hydrauliska konduktivitet.
4. Storleken av nettotillförsel av vatten till torvmarkens yta.
5. Den säsongsvisa variationen av nettotillförsel av vatten.

Resultaten visade främst att det är det lager som har den lägsta hydrauliska konduktiviteten som är mest betydelsefullt för hur flödesmönstret bildas och blir bestämmande för flödets storlek. Det kan antingen utgöras av ett ler- eller gyttjelager under torven eller av ett höghumifierat torvlager. Förekomst av sprickor eller försvagningar i ett sådant lager kan öka flödet och transporten av lösta ämnen in i torven väsentligt. Den största tillförda mängden uppkom när sådana sprickor förekom i starka utströmningsområden. Å andra sidan noterades att ett lösligt ämne kunde spridas effektivt också om sprickorna förekom i områden med mindre flöden. Högre koncentrationer i torven vid sådana situationer än vid större utflöden kan bero på att starka utströmningsområden också utgjorde utströmningsområden för torvmarken, vilket innebar att spridningen in i torven blev mindre.

Om ett tätt lager förekommer blir betydelsen av ett andra tätt lager liten. Betydelsen av horisontella genomsläppliga lager blev också begränsad, liksom effekten av anisotropi, där horisontella konduktiviteten gavs ett hundra gånger högre värde än den vertikala. Anledningen till dessa resultat torde vara att den horisontella flödesgradienten som utvecklades i simuleringarna blev avsevärt mindre än den vertikala.

Även om vertikala gradienten var betydligt större än den horisontella, visade simuleringarna att torvmarkssystemet är mycket känsligt för små förändringar i grundvattenytans läge. En måttlig förändring i nettonederbörden kan leda till stora förändringar av flödesmönstret. Simuleringar som tog hänsyn till normala säsongsvariationer visade sig dock inte ge någon större effekt jämfört med ett genomsnittligt flöde, men mer långvariga variationer ger sannolikt klara skillnader i flöden. Betydelsen av flödesriktning avtog dock starkt vid förekomst av täta lager, eftersom diffusionsprocesser då tog över ämnestransporten från den advektiva transporprocessen.

Contents

1 Introduction

In SKB's work towards a safety assessment report, mires are recognized as potentially important recipients for radionuclides /SKB 2004/. In current model approaches for dose assessments, peatlands are represented by a single box model where incoming water gets continuously mixed, with exchange between water and solids determined by a distribution coefficient (K_d) and substrate concentrations /Karlsson et al. 2001, SKB 2004/. Thereby, the concentrations get homogeneously distributed within the peatland. However, most studies of peatlands indicate some spatial variability of dissolved and sorbed substances /Kellner 2003, Lidman 2005/. The geological settings of peatlands also include variable combinations of materials with a wide range of hydraulic properties. In combination with that, different hydrological settings could result in a range of flow patterns and in various distributions of substances. Therefore it is important to examine if distributions of substances become different in more realistic (distributed) descriptions of water flow in peatlands.

There is a variety of different peat types. Development of a peatland over time with shifting vegetation covers is a common cause to the fact that there are different horizontal layers with quite different properties. These are characterized by different mother plants and different degrees of decomposition. The variation in properties results, among other things, in different hydraulic conductivities (k), which may influence the groundwater flux through the peatlands significantly, and thus cause a very complicated distribution of substance concentration within peatlands. In spite of their often flat appearance, peatlands can also be in positions of various hydraulic-head gradients, and can in fact also create hydraulic-head gradient variations themselves by peat accumulation /Kellner 2003/.

The intention with this report is to examine in what extent the variation of hydraulic conductivity within a peatland and adjoining sediments would affect the flow patterns within it under some certain hydraulic-head gradients and other certain border conditions. The first part of the report contains a short review over organic and mineral-soil sediment types and characteristics and what we know about present peatlands and underlying sediments today. In the next part, a 2-dimensional model is used to simulate flows and transports in different settings of an imaginary peatland. The objectives of the modelling work presented in this report are to study the effects of some particular factors. The specific studies of the following factors are described in separate sections of the report:

1. The magnitude of the hydraulic conductivity of the peat and of underlying layers.
2. Presence and positions of cracks in underlying clay layers.
3. Anisotropy and heterogeneity in peat hydraulic conductivity.
4. The size of the water recharge at the peatland surface.
5. The seasonal variation of the water recharge.

2 Peatland soil layers and hydraulic complexities

2.1 Different types of peat

Peat is normally classified according to its appearance, state of decomposition and vegetation type of the mother material of the dominating species (and peatland type). The qualitative descriptions of the different peat types used here are mainly obtained from /von Post and Granlund 1926/. They formulated a system that attempts to describe peat in quantitative terms by dominating plants, degree of humification, water content, presence of fine fibres and coarse fibres and wood remnants.

This classification was primarily created in order to identify the properties of the surveyed peat for use as burning fuel. The classification also tells about the historical development of the peatland and the different stages and conditions in the past. It is consequently widely used also by ecologists and paleoecologists /Clymo 1983/, but also for engineering purposes and for identification of physical properties /Hobbs 1986/. The basis for this classification system is the type of mother materials, including descriptions of the dominating plants /von Post and Granlund 1926/. The peat classes constitute two main groups: fen peats and bog peats.

2.1.1 Fen peats

Phragmites peat: Sometimes pure root mat of *Phragmites* (reed) but mostly mixed with clay and gyttja. From low to medium humified, presence of low-humified roots makes the layers less dense. *Cladium* peat is similar to *Phragmites* peat but is generally more humified.

Carex peat: Can vary from almost non-humified root mats to a more or less decomposed mass.

Brown moss peat: Similar to *Carex* peat but where brown mosses dominate over sedges.

Fen mud is a variant with dense, highly humified sediments with intermixed sedge roots, formed by sedge communities in loose deposits where plant residues get highly humified by oxygen-rich conditions.

Broad-leaf fen peat is similar to fen mud, but contains pieces of wood. It is always highly humified.

2.1.2 Bog peats

Cuspidatum bog peat, *Carex-Sphagnum* peat: Formed in wetter areas of poor fens and bogs, often with a low degree of decomposition, dominated by *Sphagnum* mosses with roots and stems of *Eriophorum vaginatum* and *Scheuchzeria palustris* or root mats of *Carex spp*.

Fuscum bog peat: Characterised by *Sphagnum fuscum* or *Sphagnum magellanicum* and plants such as *Eriophorum vaginatum, Trichophorum cespitosum* and *Calluna vulgaris*. Degree of decomposition varies a lot, from highly humified to very low humification.

Pine bog peat: Woody bog peat, formed by pine (or birch) bogs, mostly highly humified, dominated by *Sphagnum spp., Eriophorum vaginatum* and *Ericaceae shrub*, but characterised by tree stumps.

2.2 Development of peatlands and resulting layering

Paludification and terrestrialisation are two different ways of peatland development. Peatland filling in lakes (terrestrialisation) /von Post and Granlund 1926/ is probably the most common type of peatland developments in the areas around the investigation sites. Peat growth directly on ground (paludification) may also occur, both as a first establishment on low, flat land rising up from the sea and on soils with bad drainage, and as a second-order feature of already established peatlands where they expand laterally as surrounding mineral soils get wetter.

Terrestrialisation can occur as lake-bottom plant communities grow and collect sediments, turning the water more shallow, and finally can more terrestrial plant communities colonize and grow there. The peat layers then follow some bottom-up order with more limnic character in the bottom with *Phragmites* peat, followed by *Equisetum* and then sedge-fen peats, likely overgrown by bog peats. Terrestrialisation can also come about as a result of filling in from floating mats. These often develop from the margins as peat forms along the shorelines or if there is a peatland bordering the lake. The floating mats are often dominated by *Sphagnum*, and they fill in the lake from top, meaning that bog-like peat could be deposited directly at the lake bottom (with some mud layer in between), as the weight of the growing peat is pushing the lower parts downwards /Sjörs 1983/.

2.3 Typical peatlands at the investigation areas

Both the Simpevarp area and the Forsmark area are situated in regions where most peatlands are formed from terrestrialisation of lakes (Swedish: "fornsjöområde") /von Post and Granlund 1926/. Current investigations in the Forsmark area /Bergström 2001, Fredriksson 2004/ indicate that most peatlands are shallow, developed from old lake sediments. During the process of land uplift the costal waters of the Baltic Sea continuously got more and more shallow. Finally the water became stagnant and shallow enough to start establishment of sediment-rooted vegetation and a terrestrialization forming the present peatland /Fredriksson 2004/. In most examined peat profiles, a thin layer of *Phragmites* peat is present at the bottom, above a layer of gyttja of varying thickness. Over the *Phragmites* layer, mostly fen *Carex* peat of shifting degree of humification or more humified fen wood peat were found.

At one extensive peatland (an open bog), /Bergström 2001/ found *Sphagnum* peat directly above the *Phragmites* layer in what was previously open water. In the same peatland she also found relatively thick layers of fen-wood and *Phragmites* peat in areas that presumably had been more sheltered. A parallel can then be drawn to current lakes in the area that often are bordered by zones of reed wetlands and wooded fens, while still open in the middle. Depending on the size of the lake and its supply of water, the central parts of the lake subsequently fills up with bog or fen peat. The most common final stage of the peatlands in this area is probably a pine bog.

/Bergström 2001/ did not mention any degrees of humification in her study. /Fredriksson 2004/ found that the wood-fen peat was usually highly humified but the degrees of humification in the *Carex*-fen peat varied independently among the profiles within the same peatland, indicating a variation in conditions for decomposition. Thus peat properties not only vary between horizontal layers, but also laterally.

2.4 Properties of peat

Some types of organic sediments have characteristic properties while others vary much with e.g. degree of humification (Section 2.1). Not much is known about how much they differ in sorption characteristics, although we might suspect that sorption capacities increase with degree of humification as the content of humic acids increases /Bergner et al. 1995/.

The hydraulic properties of peat have both been found to vary among and within the different peat types. The permeability (hydraulic conductivity) is closely related to the pore-size distribution and the presence of large and continuous pores. The occurrence of large pores in peat can be described to vary with different factors, such as /Ingram 1983/:

- Botanical composition, with the general order from the least to the most permeable: Sphagnum moss < Carex sedges < Phragmites.
- Degree of humification (decomposition), with an increase in the degree of decomposition leading to both a larger fraction of fine material (fine pores) and a deterioration of the structure of larger pores.
- Bulk density, where an increase in bulk density often is related to increased compaction, which decreases the fraction of large pores.
- The void ratio, which can be seen as the reverse of bulk density; perhaps the readily drainable void ratio or porosity is more usable, since it is a direct measure of the amount of wider pores offering small resistance to water flow.

Although there are some studies that have found significant differences between different types of peat e.g. /Päivänen 1973/, the importance of the degree of decomposition and bulk density have been shown to be larger. The surface layer of peatlands is often only little compacted and decomposed, leading to large fractions of large pore-diameter peat. Thus, it is highly permeable. Bog surface layers are generally more permeable than those of fens, as the more eutrophic conditions of fens favour more rapid decomposition /Hobbs 1986/.

Measured saturated hydraulic conductivities in layers below 10 cm depth range between 10^{-8} and 10^{-3} m s^{-1} (for a summary of published measurements, see e.g. /Kellner 2003/). In the upper decimetres of the peat, k often decreases sharply with depth since there is a strong increase in the degree of decomposition and bulk density at those depths. However, k can vary independently of depth in the lower layers. This is because the humification process is much slower and the relative change in stress with depth is small, which causes smaller increases in compression (i.e. in bulk density). Thus, the character of the peat at larger depths is to large extent determined by its condition when it passed the upper layers, where the more efficient aerobic decomposition processes were active.

The peat is more decomposed at some depths than others because, for instance, the climate was drier at the time when this layer was at the surface, while other layers, deposited in more water-logged conditions, are much less decomposed. Even individual layers are often more or less heterogeneous. Plant root tufts often result in patches of more decomposed peat since they create oxidized zones around the roots, leading to higher bacterial activity there and consequently more efficient decomposition. Continuous root mats can therefore be very tight and have been found to act as barriers with big differences in hydraulic head at each side /Romanowicz et al. 1993/. On the other hand, some *Phragmites* and *Cladium* root mats have been found to be very permeable with $k > 10^{-3}$ m s^{-1} /Baird et al. 2004/.

2.5 Underlying sediment conditions

In simulations of groundwater flows and transports within a large peatland, /Reeve et al. 2000, 2001/ showed that the properties of the underlying mineral soils were important for determining the flow paths. Hence should not only the distribution of peat properties be of potential importance but also the border conditions of the peatland, i.e. the hydraulic conductivity of the underlying mineral soils.

Terrestrialisation peatlands are often lying on clay and gyttja soils, since clay and gyttja often get deposited as sediments in calm waters that eventually turn into peatlands. The clay is mainly deposited as glacial sediments with possible subsequent reordering and sedimentation (postglacial sediments). Gyttja, on the other hand, is deposited as organic sediments from sea and lake organisms. There is often a thin layer of sand or gravel between the clay and gyttja layers, as a result of outwashing from the glacial deposits in connection with land rise above sea level. /Hedenström 2004/ presented a generalized stratigraphy of the water-deposited sediments in the Forsmark area, from freshwater-lake deposits at the top to glacial sediments at the bottom: calcareous gyttja, algal gyttja, clay gyttja, sand and gravel, postglacial clay, glacial clay.

Often, thick (> 1 m) gyttja sediments are found in lower parts of the lakes, overlying clay gyttja of shifting thicknesses, while only thin or no gyttja is found at local heights and other exposed surfaces /Bergström 2001/. The thickness of the clay layer depends on the conditions for sedimentation and subsequent conditions during the land uplift. On more exposed surfaces the fine materials get washed out, leaving only coarser grains in the remaining sediments. Hence, it is plausible that the clay layers are less profound in the shallow areas. In the investigation areas, clay layers are also shallower or absent in areas affected by erosion. Also in near-shore areas of today, till and other coarse-grained deposits dominate /Hedenström and Risberg 2003/.

Clay can normally be treated as a low-permeable soil type ($k \approx 10^{-8}$ m s^{-1}), while the properties of a silty or gravely sand layer can shift from rather permeable ($k \approx 10^{-4}$ m s^{-1}) to more dense ($k \approx 10^{-6}$ m s^{-1}), and even low-permeable if the particle size is not homogeneous and fine sediments are intermixed /Freeze and Cherry 1979/. The hydraulic properties of gyttja are not very well known. Similarly to peat, it seems that the gyttja soils can have various structures /von Post and Granlund 1926/, with coarser materials intermixed with finer in various extents and the available descriptions are not designed for hydraulic properties. The hydraulic properties can probably be assumed to depend on the porosity or degree of compaction, but there are very few published measurements on lake sediment hydraulic properties and soft-bottom fluxes.

The flow of water in or out of lakes generally decreases with distance from shoreline /Shaw and Prepas 1990, Kishel and Gerla 2002/. Although the cause of this relationship can both be a decreased hydraulic conductivity and decreased hydraulic gradients, the hydraulic conductivity is likely lower in parts protected from erosion and where sedimentation conditions have been favourable. /Kishel and Gerla 2002/ found hydraulic conductivities to vary between 10^{-6} and 10^{-4} m s^{-1} in a 1 m thick "organic sediment" layer just outside the shore line of a small lake. In a study of a peatland-pond system, /Ferone and Devito 2004/ found k values of 10^{-7} m s^{-1} in gyttja deposits just below water column/peat layers, decreasing to less than 10^{-8} m s^{-1} in deeper layers.

/Bergström 2001/ investigated the taxa of the gyttja sediments in the Forsmark area, and her studies of water content suggest porosities of more than 95% in the algal gyttja sediments. /Hedenström and Risberg 2003/ also present high values of water content, although decreasing with depth. There is reason to believe that the gyttja gets compressed under peat so its hydraulic properties probably change during consolidation in the transfer from lake sediment to peatland bottom. Thus, we could expect gyttja under peat to have a low hydraulic conductivity.

2.6 Aspects of modelling the flows in a peatland

Despite the similarities in the general settings, the present site investigations indicate a variation in peat properties that may become hard to predict or simulate without large uncertainty. The heterogeneity and the fact that so many factors apply in the formation of peat, make it hard to develop general peatland development models that apply to different settings and shifts in climate. In addition, the uncertainty of the relationships between peat type and the size of hydraulic conductivity can cause errors of several orders of magnitude in k values in a certain area.

Since an increase of detailed information would also contain these sources of uncertainty, one can claim it justified to use flow models without much spatial details in their descriptions. On the other hand, it is still uncertain what kind of effects we would expect from different variations. Therefore a model study, with the aim to understand the effects of some layer orders within a certain range of variability, is well motivated because it can help to point out the necessary studies and model developments that have to be made.

2.6.1 Distributed flow in peatlands

A more realistic model than a box model would include distributed descriptions of flows and transports. Unfortunately, not much is known about the flow patterns in peatlands. The flow paths in peatlands have until recently been assumed to depend on surface-layer hydraulic heads, following the concept by the assumption of Dupuit-Forcheimer /Ingram 1983/, which means that the flow is uniform in the direction of the slope of the water table /Freeze and Cherry 1979/. However, this type of description has shown to be too simple. This is clear at peatland settings located in discharge zones, where the vertical flows are of the same size as the horizontal.

Where bogs develop, the higher hydraulic heads at their centres e.g. /Kellner 2003/ can develop vertical flows, directed downwards in the centre (recharge zone) and upwards in the outer areas (discharge zone). /Price and Woo 1990/ showed that local recharge-discharge processes have to be considered to get concentrations corresponding to measured values, whereas only diffusion could not explain the concentration patterns. /Reeve et al. 2001/ showed how mechanical dispersion could be responsible for measured concentration distributions in large bog-fen systems where the dominating flow is horizontal. However, /McKenzie et al. 2002/ showed that vertical flow influences pore-water chemistry in domed bogs by advective transport. Hence, it seems necessary to describe the groundwater flow pattern correctly.

Increasing the complexity of a model from a single box into a more distributed flow description, the first step would be to have a homogeneous peat deposit but with distributed applied heads. The next step would be to study the importance of k in the underlying sediments. The importance of a tight underlying layer can then differ between situations with high and low k in the peat for example. There could also be local high-impact points where there are breaches in a tight layer. For example there may be similar effects as observed in peat around crack zones in the underlying igneous bedrocks, which have yielded enhanced contents of minerals /Fredriksson et al. 1984/.

2.6.2 Heterogeneity and anisotropy

A potentially important factor is the distribution of the hydraulic conductivity within the peat itself. From the preceding Sections 2.2–2.4, it is clear that we can almost always expect some kind of layering, although the details would be uncertain. The non-uniform properties can be manifested in two entities, heterogeneity (differences in permeability among different localities) and anisotropy (difference in permeability along different directions within the same locality). The heterogeneity can simply be because there is a spatial variation of peat types as described in Sections 2.2–2.4.

Anisotropy has been found in many peat samples, although not many adequate studies of the magnitudes have been done. /Chason and Siegel 1986/ found in a laboratory study that most of their data pointed towards a greater horizontal k than the vertical, although there was a great spatial variation in the anisotropy. /Beckwith et al. 2003a/ found in a laboratory study that horizontal k was greater than vertical k in most of their bog-peat samples with a mean anisotropy (k_{hor}/k_{ver}) of 4.

An interesting point is that the heterogeneity associated with the layering that normally develops, with fewer and more permeable layers, also brings about anisotropy, in the larger scale perspective. One must then remember to adapt results from k measurements, which are often of the scale of decimetres, when models with grid cells in a much larger scale should be parameterized. The results also might depend on the scale of the model (or actual peatland) with respect to the hydraulic-head gradients in different directions. Therefore, it is motivated with a model study on the scale of a moderately sized peatland.

In a small-scale modelling study (1.1 m in length) /Beckwith et al. 2003b/ studied effects of heterogeneity and anisotropy, based on their laboratory measurements of these parameters /Beckwith et al. 2003a/. They found that heterogeneity and not anisotropy had the greater influence on the complexity of groundwater flow. /Chason and Siegel 1986/ suggested that the layer with the largest k would have the largest influence on transport, but /Beckwith et al. 2003b/ concluded that it was rather the transport ability to this layer that should be the most important. In other words, it could be the least permeable layer that determines the flow and solute transport.

2.6.3 Temporal variation in hydraulic heads

When it comes to the hydraulic-head gradients that drive the flows through a peatland, the hydraulic-head differences are often found to be small. This leads to high sensitivity to changes, and just a minor raise in a fen water table may lead to a switch towards downward flow inducing bog development /McNamara et al. 1992/. In several studies, seasonal shifts in hydraulic-head gradients have been observed with upward-directed gradients during dry periods with declining water table and downwards-directed gradients during wet periods /Siegel and Glaser 1987, Romanowicz et al. 1995/. There are several possible explanations for these, such as underlying aquifers with a more stable hydraulic head than the water-table variation, presence of low-permeable layers between upper and lower zones and atypical pressure changes, e.g. gas formation, in the lower zones. A simulation of the seasonal variation of the surface-water recharge would help to understand its importance and what the net effect would be.

2.6.4 Properties considered significant to study

Given the different aspects mentioned above, it was decided to make simple simulations of a smaller peatland to examine the influences of the following characteristics:

1. The magnitude of the hydraulic conductivity of the peat and of underlying layers.
2. Presence and positions of cracks in underlying clay layers.
3. Anisotropy and heterogeneity in peat hydraulic conductivity.
4. The size of the water recharge at the peatland surface.
5. The seasonal variation of the water recharge.

3 Model description

In the modelling work of this report, the software package HYDRUS-2D /Šimunek et al. 1999/ was used. HYDRUS-2D incorporates a finite-element model for simulating water, heat and solute movement in two-dimensional variably saturated media. Here, water and solute movement (not heat transport) were simulated. Water flows are calculated by using Richard's equation while the convection-dispersion equation is used for solutes. More details on the parameters of this model are given in appendix.

A 2-dimensional flow model domain was considered. The length was 300 m and the depth 12 m. A bowl-shaped peatland was located in the middle of this landscape element. The peatland was 150 m wide at the surface, and 100 m at its bottom, which was at 4 m depth. The geometry was described with a rectangular grid, consisting of 40 vertical columns and 26 horizontal rows. The grid size varied as the grid cells were smaller in the parts of the model with dense sediment layers, with cell size of 2.5×0.2 m^2, than in the peripheral parts where the largest cells were 20×1.0 m^2.

Five different material "layers", described in Table 3-1, were applied in the model (Figure 3-1). The first material from the top represented the peat. The second material had similar properties to the peat, i.e. organic material, but was given in a separate layer as to allow a layer with different hydraulic properties resembling for instance a gyttja layer. The third and fourth materials were set as mineral soil layers with hydraulic properties shifting from high to low permeability (representing sandy and clay layers). The fifth material was the basic material of the model, representing a surrounding aquifer with highly permeable soil. The basic material in the flow domain was given a relatively high hydraulic conductivity, 1×10^{-4} m s^{-1}.

Two types of solute were injected along the borders of the model. One type was highly adsorptive while the other was a non-adsorptive. Both solutes were non-reactive; details are given in Table 3-2. The intention with this model setup, with a larger aquifer surrounding the peatland, was to allow the solutes to easily reach the borders of the sediments, but instead of putting the border conditions directly at the lower/outer parts of the sediments this setting allows the flows and heads of the peatland to interact dynamically with the underlying soil. Some properties of the five materials were constant (Table 3-1) whereas other properties varied among the different simulations.

Table 3-1. General properties of materials in simulation model.

Soil number	Soil type	"Effective porosity"	Dry bulk density (kg/m^3)	Longitudinal dispersivity (m)	Transversal dispersivity (m)	Adsorption coefficient, solute 1 (m^3/kg)
1	Organic	0.5	200	0.1	0.01	10
2	Organic	0.5	200	0.1	0.01	10
3	Mineral	0.4	1,500	0.5	0.01	0
4	Mineral	0.4	1,500	0.1	0.01	0
5	Mineral	0.4	1,500	0.1	0.01	0

Table 3-2. Properties of the two solutes injected into the model.

Solute number	Type of solute	Injected concentration (mol/m^3)	Molecular diffusion coefficient (m^2/s)
1	Adsorptive, instant	1.0×10^{-3}	1.0×10^{-9}
2	Non-adsorptive, conservative	1.0×10^{-3}	1.0×10^{-9}

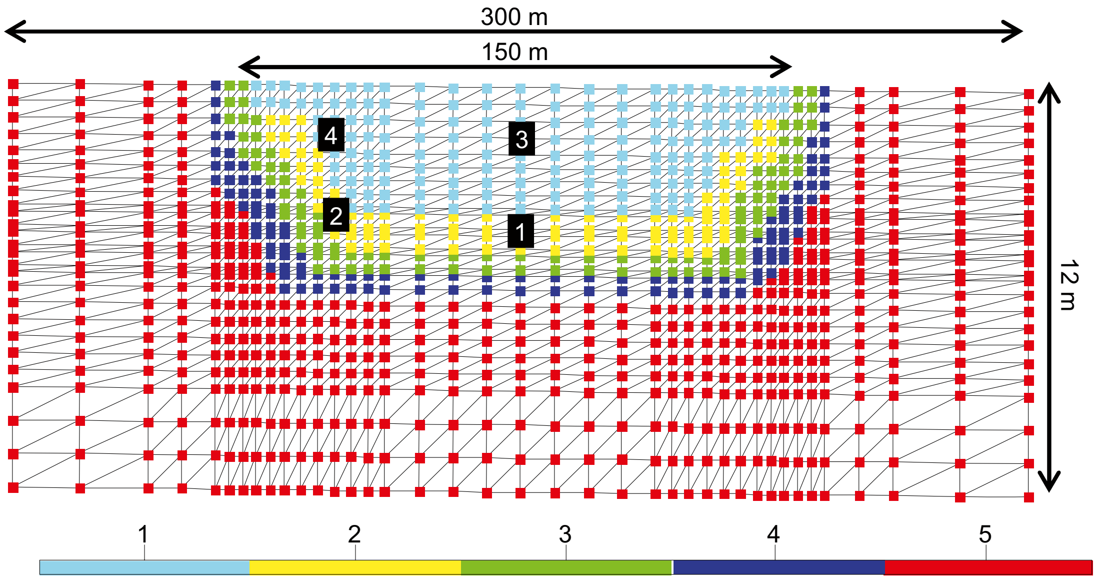

Figure 3-1. *The two-dimensional flow domain of the model with the finite-element mesh represented by dots and lines. The different colours 1–5 denote the five different materials in the model as described in text and Table 3-1. The numbered squares denote the four observation points for which the temporal variation in solute 2 will be reported.*

The values of "effective porosity" in Table 3-1 are derived from applied model parameters of the pore-size distribution, described in Appendix, more representing the drainable porosity than the pore volume participating in the flow. Dual porosity effects are not explicitly taken into account. Dispersivity values are based on results from column experiments, yielding longitudinal dispersivities of 2 mm to 10 cm /Hoag and Price 1997, Ours et al. 1997/. Transversal dispersivity was chosen to be 0.1 times longitudinal dispersivity, in accordance to the study of /Reeve et al. 2001/.

The adsorption coefficient values are chosen to represent a substance similar to Uranium in organic soil (distribution coefficient about 10,000 L/kg) for the adsorptive solute but in mineral soil it is chosen to be zero because the intention was to study only the transports in the organic material. The descriptions and concentrations of the solutes are given in Table 3-2. The molecular diffusion coefficient values are obtained from /Reeve et al. 2001/.

The relation between advective and diffusive transports can be described with the Peclet number, *Pe*, which is calculated as:

$$Pe = {}^{vL}\!/_{D}$$

where v is water velocity, L is characteristic length and D is diffusion coefficient /Clark 1996/ and $Pe >> 1$ represents a dominance of advective transports while $Pe << 1$ characterises diffusive transport dominance e.g. /Clark 1996/. If $L = 1$ m, $D = 10^{-4}$ m^2 day^{-1}, and $v = 0.01$ m day^{-1} are assumed, Pe becomes 100, which can be considered much more than 1, while $v = 0.0001$ m day^{-1}, which is more representative for a tight layer, produces $Pe = 1$.

4 Effects of the hydraulic conductivities of peat and underlying layers

The influence of the permeability of the bottom sediment was studied with varying values of the hydraulic conductivity in the peat layers. The bottom sediment layer can consist of a tight soil such as clay. The bottom sediment could also consist of a permeable soil. The condition constituted by this layer may be of great significance, and thus it is important to investigate its influence. The study consisted of 12 simulations.

4.1 Common settings among simulations

There was a general flow of water along the model with a slope of 1%. Constant head was applied at the sides and the bottom of the flow domain. The heads were in hydrostatic equilibrium at each side and with the bottom, such that the general slope in head was the same as the model slope. A constant head was also applied at the surface of the central part of the domain, representing the peatland (Figure 4-1). Two types of constant head were applied at the surface: one with zero pressure, meant to represent a flat fen with upward hydraulic gradient. The other type had a positive pressure increasing from zero at the borders of the peatland to 1.0 m at the centre, representing a bog mound. For every set of material distribution both a bog and a flat fen situation were simulated.

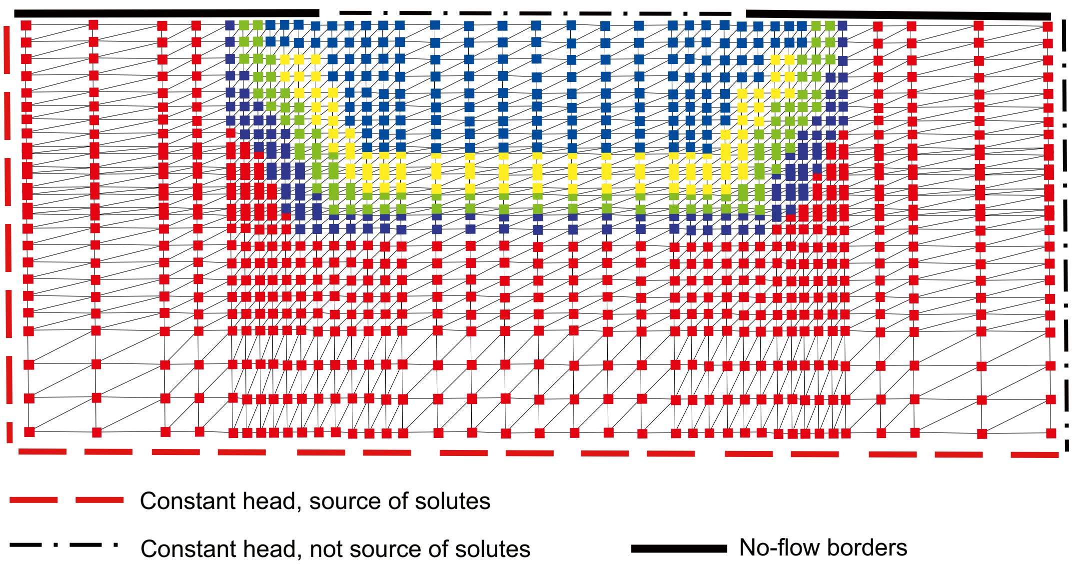

__Figure 4-1.__ Common border conditions for the first simulations. The flows were driven by constant-head boundaries. The heads were in hydrostatic equilibrium at each side and with the bottom, such that the general slope in head was the same as the aquifer slope, i.e. 1% from left to right. The pressure was 12.5 m water along the bottom, a 0.5 m overpressure. The pressure at the top constant-head border (peatland surface) was either 0 everywhere or 0 at the borders and increasing to 1.0 m at the centre. The solutes were constantly applied during the whole simulation.

4.2 Features of the individual simulations

The organic sediments, layers 1 and 2, were assumed to be homogeneous and were designated hydraulic conductivities representing either quite permeable (k = 10^{-4} m s^{-1}), intermediately permeable (k = 10^{-6} m s^{-1}) or less permeable organic soils (k = 10^{-8} m s^{-1}) /Kellner 2003/. Each of these three variants were combined with a permeable (k = 10^{-5} m s^{-1}) or a less permeable (k = 10^{-8} m s^{-1}) sediment sub-layer, layer 3. These six combinations were combined with two different applied hydraulic heads at the surface (Table 4-1), representing a fen (simulations 4.1–4.6) and a bog (simulations 4.7–4.12).

4.3 Results

The results are presented partly in a qualitative way by showing figures of velocities, concentration distributions, time plots of concentrations at certain locations, and also by presenting values of retained amounts of both solutes in the two organic layers after a simulated time of 100 years.

4.3.1 Fen-type peatlands

For an upward hydraulic-head gradient, the concentration increase rate at one point depends on the distance from the source and the hydraulic conductivity of the layers in between. The simulations with an upward hydraulic gradient (the fen type) showed an increasing concentration with time for both the adsorptive and the conservative solutes. The adsorptive solute 1 was mainly captured at the borders between organic and mineral soils, and the gradients in solute concentration became sharp in these areas.

The concentrations of conservative solute 2 became soon as high as within the source water. The rate of concentration increase was dependent on water flux rates and thus on the hydraulic conductivity. The concentration increase rate became substantially lower in the presence of a low-permeability layer with k = 10^{-8} m s^{-1}. Some type cases will be presented here:

Table 4-1. Parameter values determining the hydraulic conductivity (k) in model layers 1–4 and the vertical gradient of hydraulic head for twelve simulations.

Simulation number	Layer 1 org k (m s^{-1})	Layer 2 org k (m s^{-1})	Layer 3 min k (m s^{-1})	Layer 4 min k (m s^{-1})	Upwards (–0.5 m) *), or downwards (+0.5 m) *)
4.1	10^{-8}	10^{-8}	10^{-5}	10^{-5}	–0.5 m
4.2	10^{-6}	10^{-6}	10^{-5}	10^{-5}	–0.5 m
4.3	10^{-4}	10^{-4}	10^{-5}	10^{-5}	–0.5 m
4.4	10^{-8}	10^{-8}	10^{-8}	10^{-5}	–0.5 m
4.5	10^{-6}	10^{-6}	10^{-8}	10^{-5}	–0.5 m
4.6	10^{-4}	10^{-4}	10^{-8}	10^{-5}	–0.5 m
4.7	10^{-8}	10^{-8}	10^{-5}	10^{-5}	+0.5 m
4.8	10^{-6}	10^{-6}	10^{-5}	10^{-5}	+0.5 m
4.9	10^{-4}	10^{-4}	10^{-5}	10^{-5}	+0.5 m
4.10	10^{-8}	10^{-8}	10^{-8}	10^{-5}	+0.5 m
4.11	10^{-6}	10^{-6}	10^{-8}	10^{-5}	+0.5 m
4.12	10^{-4}	10^{-4}	10^{-8}	10^{-5}	+0.5 m

*) This number was calculated as the difference between the hydraulic head at the centre part of the peatland surface and the hydraulic head at the bottom of the model.

Type 1. Permeable fen with no clay at bottom (simulation 4.3). Here almost all the flow of water in the fen became directed vertically upwards within the fen (Figure 4-2). The water velocity was up to 6 cm day^{-1}, which gave a quick total saturation of solute 2, while solute 1 did not penetrate far from the interface with underlying mineral soil during the simulated time.

Type 2. Non-permeable fen with clay or no clay at bottom (simulation 4.1). The non-permeable peat did restrict all but very small flux in the peatland (Figure 4-3). Water velocities were in the order of µm day^{-1}. It took solute 2 about 200 years to reach full concentration in the peat, which indicates that much of the concentration increase was caused by diffusion. The inflow of solute 1 was also low and less sharp concentration gradients indicated the importance of diffusion for transport.

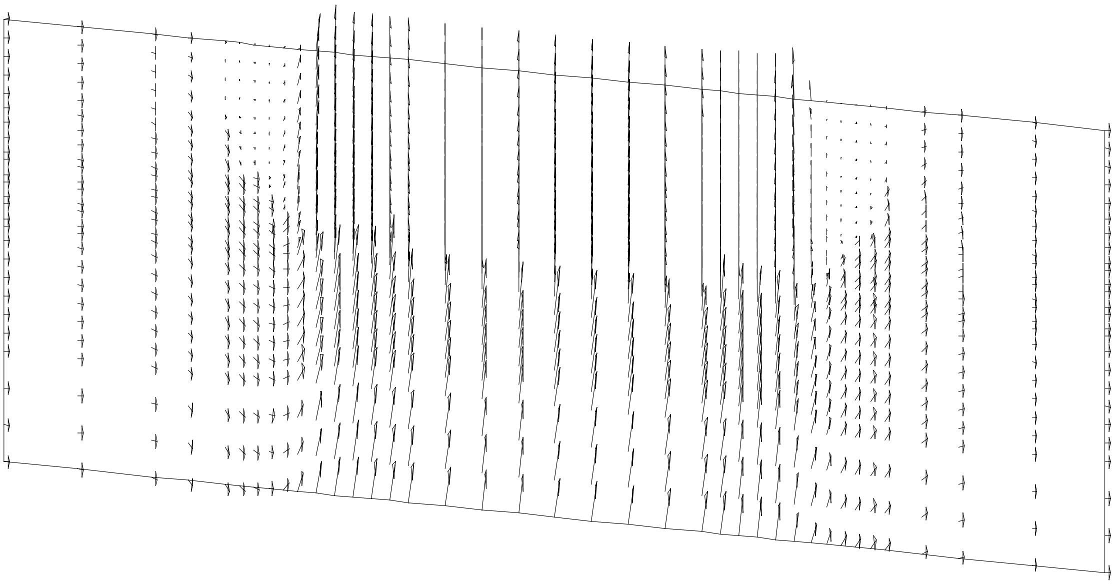

Figure 4-2. *Flow pattern in simulation 4.3 that has a model setting of a peatland with zero pressure head at the surface, and peat k =* 10^{-4} *m* s^{-1}*, situated in an aquifer with k =* 10^{-5} *m* s^{-1}*.*

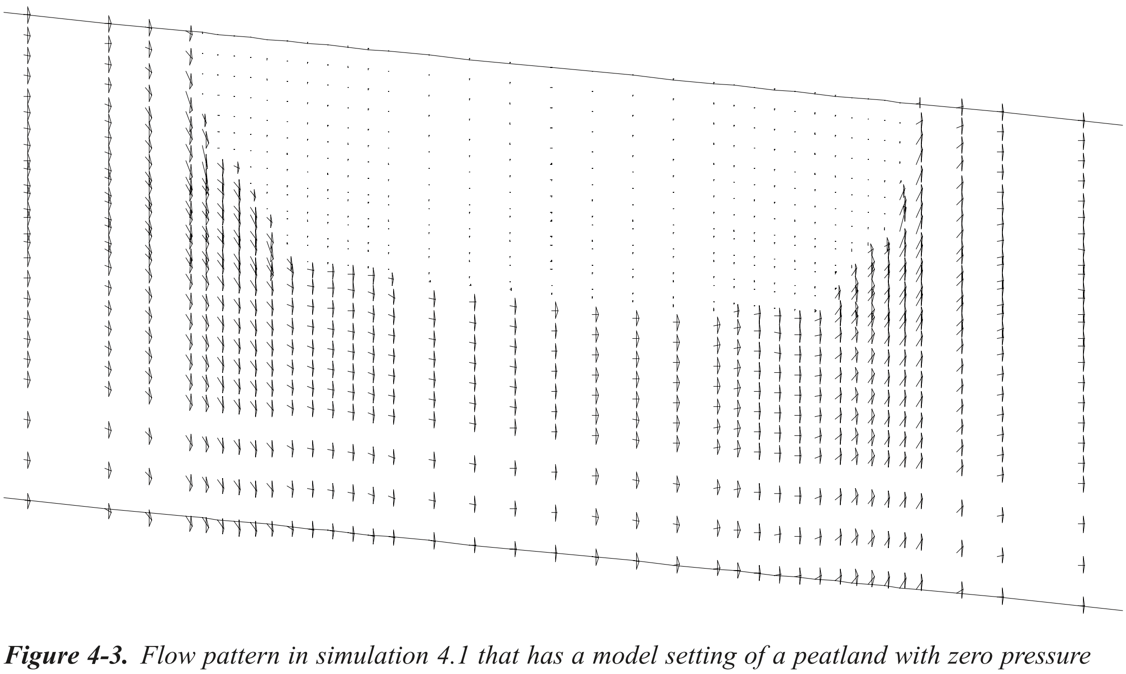

Figure 4-3. *Flow pattern in simulation 4.1 that has a model setting of a peatland with zero pressure head at the surface, and peat k =* 10^{-8} *m* s^{-1}*, situated in an aquifer with k =* 10^{-5} *m* s^{-1}*.*

Type 3. In cases with a permeable peat, the presence of a clay layer (simulation 4.6) caused significantly less vertical flow and exchange between organic layers and underlying mineral soil. When the peat permeability was high, the 1-%-slope of the model fen surface generated a local flow cell within the peat (Figure 4-4), with a recharge area at the upslope end and a discharge area at the downslope end of the peatland. This resulted in almost zero concentration for solute 2 at the recharge area and clearly diluted concentrations in the rest of the peat zones (Figure 4-5). The clay layer had less impact on the flows and transports in the less permeable peats, where diffusion flows dominated over convective flows. The presence of a clay layer in addition to a low-permeable peat (simulation 4.4) did not cause any substantial difference in the flows and transports in the peat.

The temporal variation of solute 2 at the observation points (Figure 4-6) shows that when a tight bottom layer is not present the effect of the magnitude of the hydraulic conductivity is just to delay the concentration increase until the whole peatland gets the same concentration as the

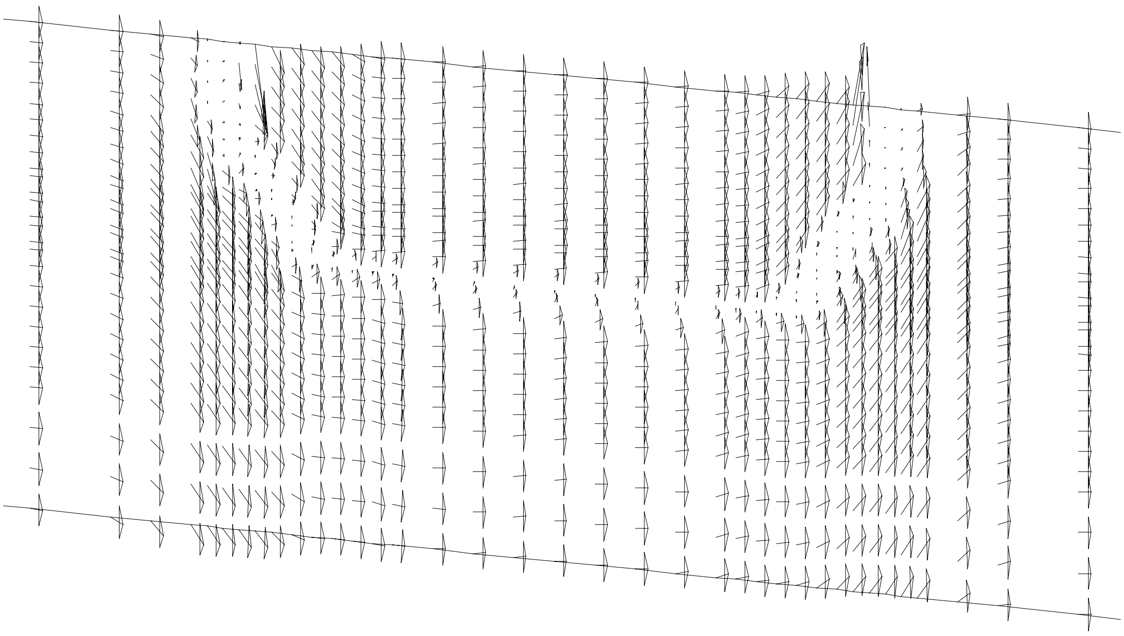

Figure 4-4. *Flow pattern in simulation 4.6, which has a model of a tight mineral-soil layer ($k = 10^{-8}$ m s^{-1}) between the peat ($k = 10^{-4}$ m s^{-1}) and the rest of the mineral soil ($k = 10^{-5}$ m s^{-1}). The arrows denote the flow direction and size of the flow at each node of the model grid net.*

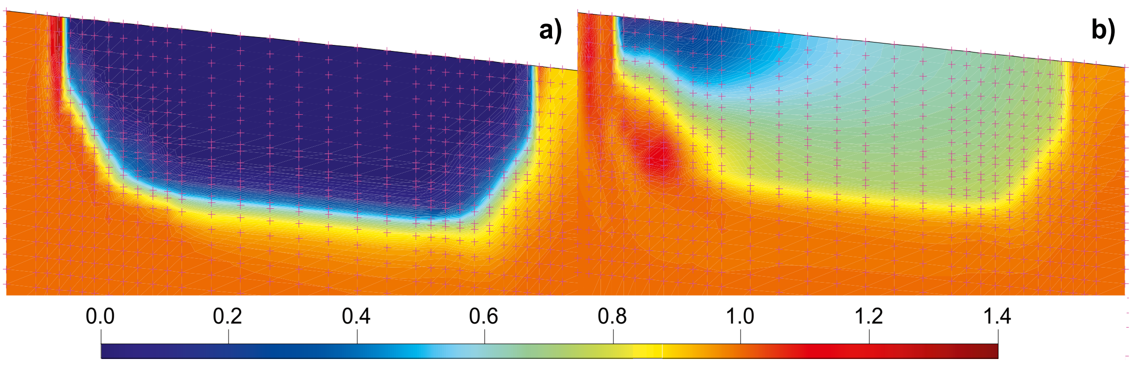

Figure 4-5. *Concentration distributions of solute 1 (a) and solute 2 (b) for simulation 4.6, which has a model of a tight mineral-soil layer ($k = 10^{-8}$ m s^{-1}) between the peat ($k = 10^{-4}$ m s^{-1}) and the rest of the mineral soil ($k = 10^{-5}$ m s^{-1}). The spectrum bar denotes the concentration of solutes in µM.*

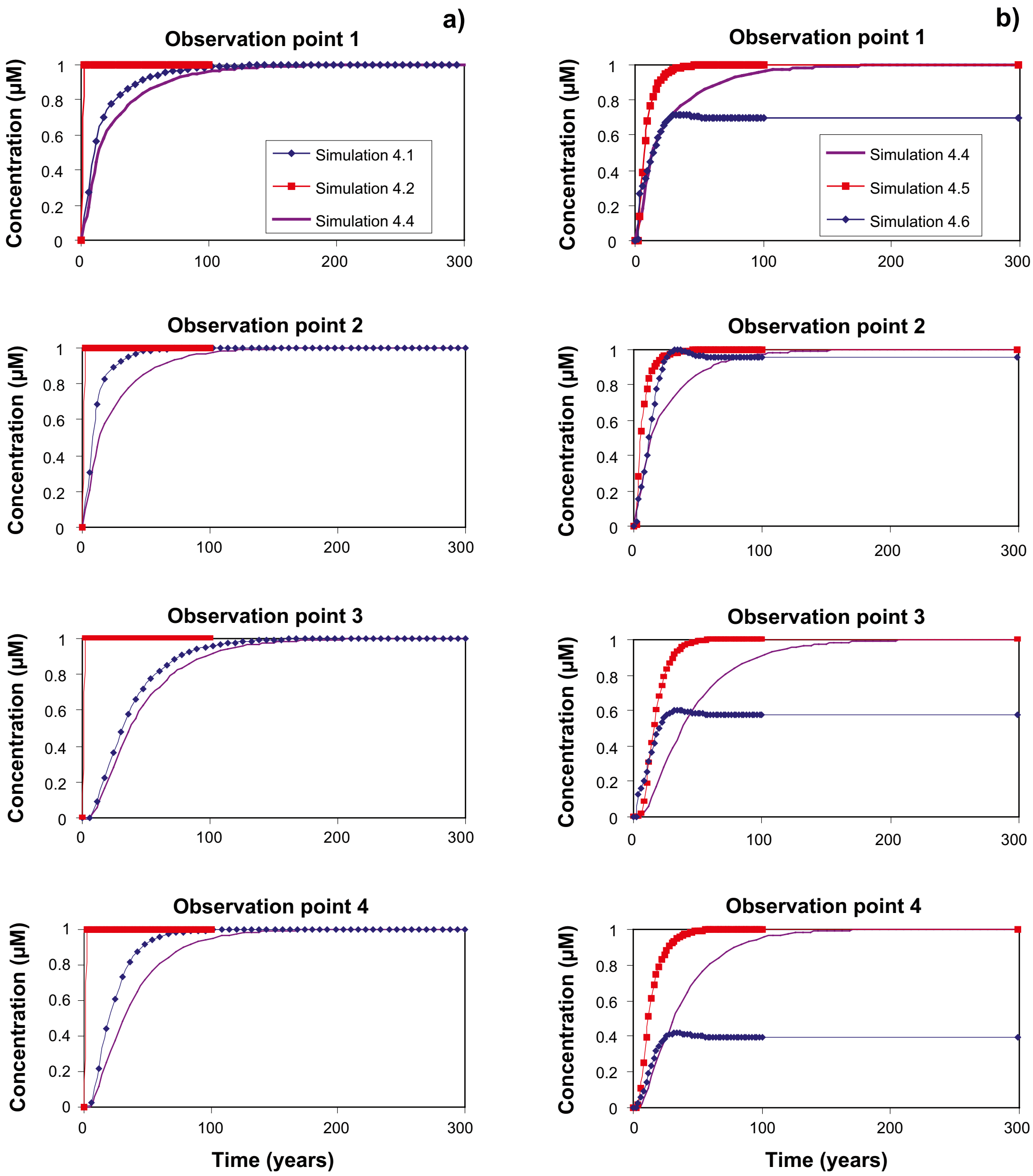

__Figure 4-6.__ Temporal variation of solute 2 at observation points 1–4 for simulations 4.1, 4.2 and 4.4 (a) and 4.4, 4.5 and 4.6 (b). Simulations 4.5 and 4.6 were stopped after 100 years because they had reached equilibrium at that point. Locations of observation points are given in Figure 3-1.

source. However, in the peatlands with tight bottom layers the effect of a permeable peat causes the water paths to change in such a way that the equilibrium concentration becomes lower at most places in the peatland.

4.3.2 Bog-type peatlands

Introducing a groundwater mound, similar to the water-table shape of a bog, affected the flow paths substantially. The low, outer parts of the bog mound constituted discharge zones similarly to the fen simulations, but the central, higher parts of the bog mound developed downward flow. In the bog simulations, this flow pattern resulted in low concentrations in the centre parts, increasing towards the outer parts. The impact of the central mound depended partly on the peat permeability. The effect of a bog mound was especially strong in the simulations with the permeable peat (Figure 4-7a). In the simulations with the permeable peat, sharp gradients in concentration of solute 2 developed between the low- and high-concentration areas, whereas the concentration gradients were less distinct in the low-permeable peat simulations (Figure 4-7b).

Similarly to the fen-type simulations, the effect of a clay layer in a bog setting was more clear in the simulation of a permeable peat than in those with less permeable peat. The results from simulation 4.12 are shown in Figure 4-8. The greater flows were kept to go within the peat layers without notably penetrating the clay, creating a local flow cell with downward directed flows in the centre parts shifting to upward discharge in the outer parts of the peatland. The higher hydraulic head in combination with the small exchange through the clay layer caused the concentrations in the peat layers to be low except at the border zones where the discharge from the bog met the discharge from the mineral soils.

The slope of the model setting created an asymmetrical flow pattern. In the central parts of the peatland the increase in head towards the centre was 0.01 mm^{-1}, which matched the general

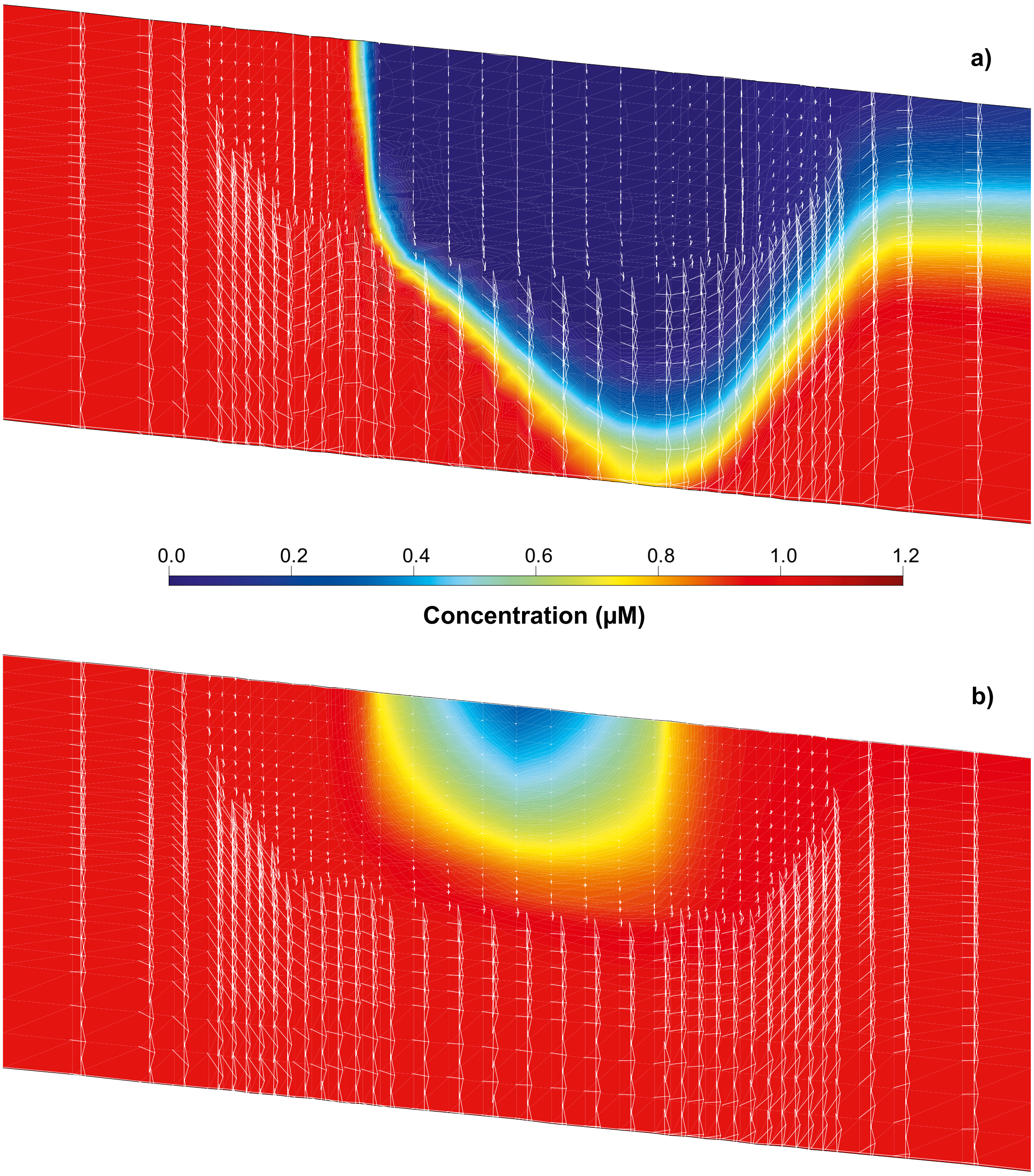

Figure 4-7. *Velocity arrows and concentrations of solute 2 after 100 years simulation time in simulation number 4.8 (a) with* $k = 10^{-6}\ m\ s^{-1}$ *and 4.7 (b) with* $k = 10^{-8}\ m\ s^{-1}$.

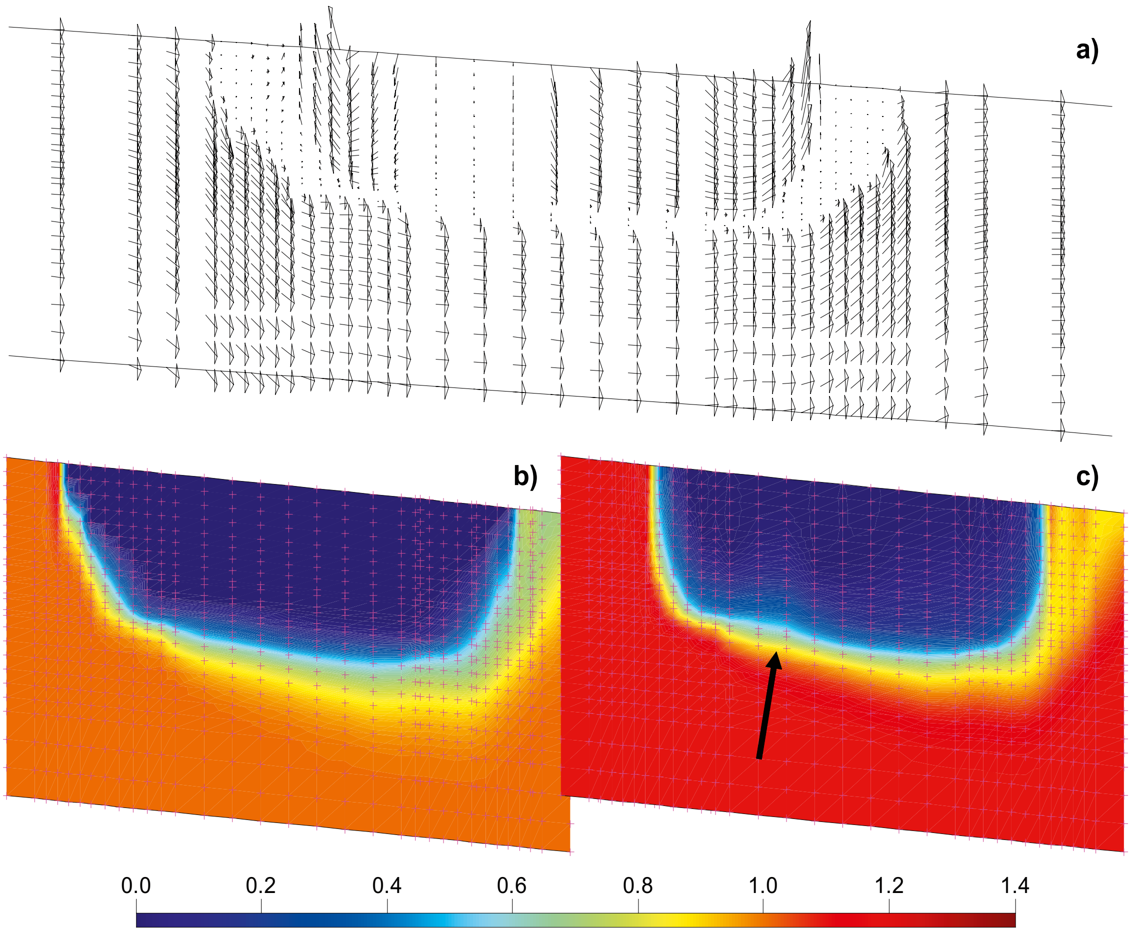

Figure 4-8. *Simulated flows (a) and resulting concentrations of solute 1 (b) and 2 (c) after 100-year simulations of a peatland with a peat mound of 1.0 m height over the surrounding ground surface, simulation 4.12. The peat k = 10^{-4} m s^{-1}, whereas the layer underneath was low-permeable (k = 10^{-8} m s^{-1}). The low flow velocities in the central left part of the peat facilitated impact of diffusive transport (as indicated by the arrow). The spectrum bar denotes the concentration of solute 1 in µM. Colour codes for solute 2 are the same, but the spectrum covering 0–1.4 µM for solute 1 is only covering the range 0–1.2 µM for solute 2.*

slope of the aquifer. This caused a very small flow in the left part where the general model slope and bog mound slope counteracted each other, and an extended head gradient towards the right in the right part where these slopes acted together. In the parts of the left side where the resulting flow rate became very small, effects of diffusion could be seen (Figure 4-8).

4.3.3 Resulting total solute contents

Total contents in the organic layers are presented in Tables 4-2, 4-3 and 4-4. The concentrations of solute 1 in fen-type simulations increased with increasing hydraulic conductivity while the presence of a low-permeable mineral soil layer (“clay”) restricted the transport of the solute considerably. The relative effect of the “clay” layer was biggest in the highly-permeable-peat simulations and decreased with decreasing k in the organic layers.

The concentrations of solute 2 were equal to source concentration in the simulations with high-permeable soils throughout. Simulation number 4.1 with k = 10^{-8} m s^{-1} in the organic layers had slightly lower content but that was because the 100-year simulation time was not long enough to saturate the peat with the solute. Total saturation of solute 2 was reached after 200 years in this simulation.

Table 4-2. Total (and dissolved within parenthesis) amounts of solute 1 (mmoles) within model organic layers after 100 years for 6 different parameter sets for fen simulations.

Bottom mineral soil layer k (m s^{-1})	**Organic layers k (m s^{-1})** 10^{-4}	10^{-6}	10^{-8}
≥ 10^{-5}	3.11×10^{5} (77.8)	3.35×10^{4} (8.38)	633 (0.16)
10^{-8}	2.95×10^{3} (0.74)	779 (0.19)	313 (7.8×10^{-2})

Table 4-3. Total (= dissolved) amounts of solute 2 (mmoles) within model organic layers after 100 years for 6 different parameter sets for fen simulations (100% saturation = source concentration corresponds to 315 mmole).

Bottom mineral soil layer k (m s^{-1})	**Organic layers k (m s^{-1})** 10^{-4}	10^{-6}	10^{-8}
≥ 10^{-5}	315	315	305
10^{-8}	199	314	288

Table 4-4. Total (and dissolved within parenthesis) amounts of solute 1 (mmoles) within model organic layers after 100 years for 6 different parameter sets for bog simulations.

Bottom mineral soil layer K (m s^{-1})	**Organic layers K (m s^{-1})** 10^{-4}	10^{-6}	10^{-8}
≥ 10^{-5}	1.08×10^{4} (3.44)	1.59×10^{3} (0.41)	561 (0.26)
10^{-8}	401 (0.16)	269 (0.13)	284 (0.12)

When a low-permeable “clay” layer was present, the resulting contents of solute 2 did not vary among the simulations in the order of the hydraulic conductivity. Simulation 4.5 with peat k = 10^{-6} m s^{-1} showed the highest final content, although not yet equal to the source concentration; it reached this concentration shortly after 100 years. Again simulation number 4.4 with k = 10^{-8} m s^{-1} had lower content because of the low transport rates and reached the source concentration later. Simulation 4.6 with peat k = 10^{-4} m s^{-1} resulted in a smaller total content because of the local flow cell mentioned earlier that developed in this simulation.

The final contents of solute 1 decreased with decreased peat k values also in the bog-type simulations, although not so substantially as for the fen simulations. All bog-type simulations also generated lower contents than corresponding fen-type simulations. In contrast to the fen-type simulations, the highest total contents of solute 2 were generated with peat k = 10^{-8} m s^{-1} (simulations 4.7 and 4.10), because the role of diffusion dominated over the downward convective flow in these settings. The content of solute 2 in simulation number 4.12 (k = 10^{-4} m s^{-1}, with “clay” layer) was markedly lower than in simulation 4.11 with k = 10^{-6} m s^{-1}, whereas in simulations 4.8 (k = 10^{-6} m s^{-1}) and 4.9 (10^{-4} m s^{-1}), which lacked the underlying tight layer, the relationship was the opposite. This was because the lower conductivity in simulation 4.8 created a less powerful local flow cell than in simulation 4.9, resulting in less upward flow in outer areas.

Table 4-5. Total (= dissolved) amounts of solute 2 (mmoles) within model organic layers after 100 years for 6 different parameter sets for bog simulations (100% saturation = source concentration corresponds to 315 mmole).

Bottom mineral soil layer K (m s^{-1})	Organic layers K (m s^{-1})		
	10^{-4}	10^{-6}	10^{-8}
$\geq 10^{-5}$	54.6	49.1	237
10^{-8}	27.4	76.2	223

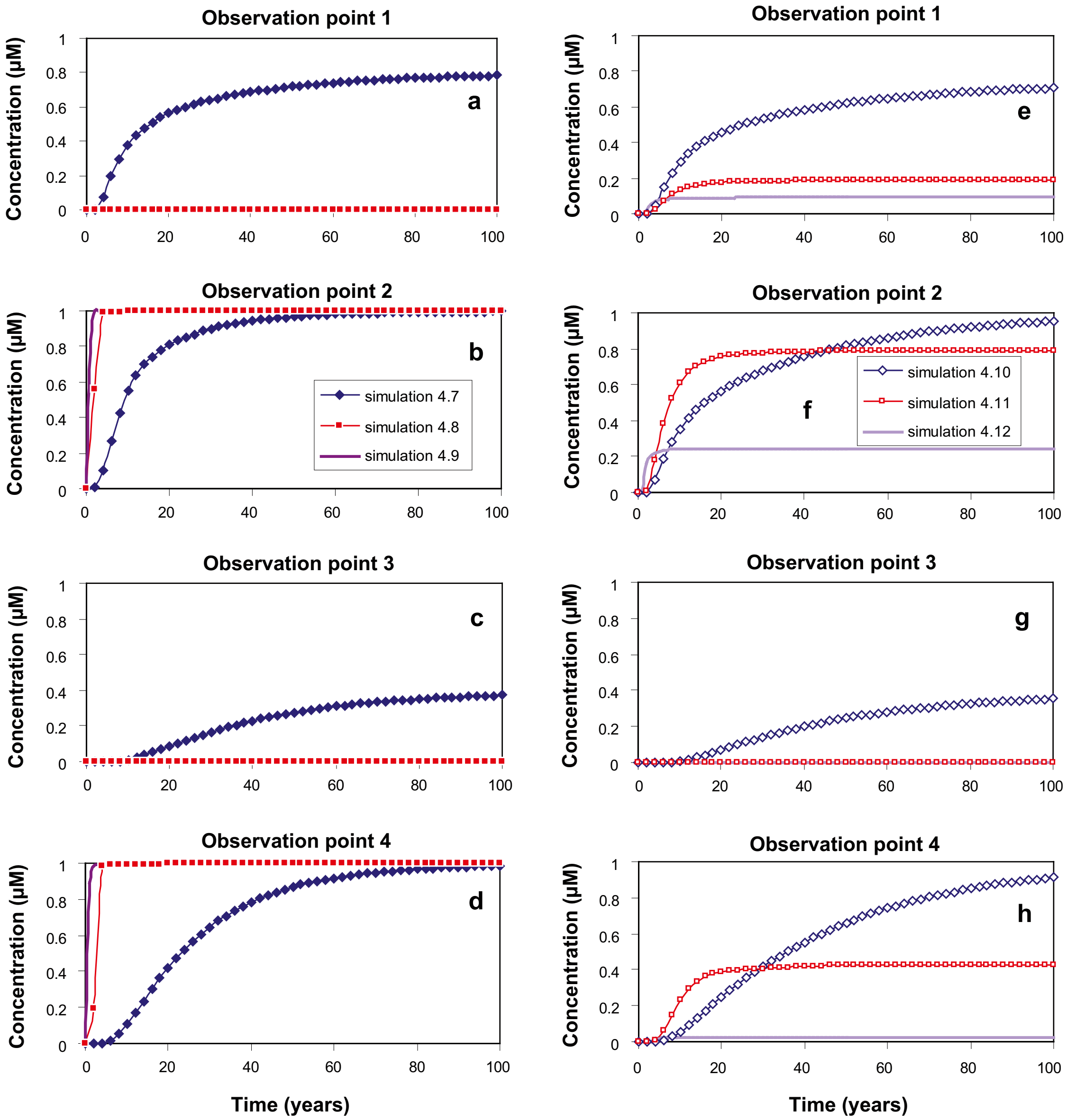

Figure 4-9. *Temporal variation of solute 2 at observation points 1–4 for simulations 4.7–4.9 (a–d) and 4.10–4.12 (e–h). Locations of observation points are given in Figure 3-1.*

4.4 Discussion and conclusions

The importance of flow direction (and hydraulic head gradient) decreases with decreasing hydraulic conductivity in the peatland. This occurs as the convective flux is slowed down and the transport is taken over by the diffusive flux. Thus the contents of both solute 1 and solute 2 in the fen-type simulations decreased with decreasing conductivity since the upward inflow rates decreased. The situation in the bog-type simulations became more complicated since the hydraulic-head mound at the bog surface created both recharge and discharge zones within the peatland. The resulting content of solute 1 was then determined by the area of solute inflow and by the flow rates, while the content of solute 2 also depended on the flow pattern primarily inside the peat layers but to some extent also outside these layers.

Presence of a low-conductivity or tight layer such as a layer of clay is an important factor. It decreases the flow and exchange of substances between peat and underlying mineral soil or bedrock and most of the transport through the layer goes by diffusive flux. If the layers above the tight layer are highly permeable, lateral gradients in these can cause local flow cells creating both recharge and discharge zones above the tight layer without any significant exchange with deeper layers.

Presence of a tight peat layer acts as an isolation towards heads on the other side of the layer. Similarly to a clay layer, a tight peat layer may act as a barrier and close off convective flows effectively while the importance of diffusive flow increases. We may assume that presence of a tight peat layer therefore can give the same effects concerning the pattern of water flow.

5 Effects of the presence and positions of cracks in clay layers

The results from the previous chapter revealed the importance of the presence of a tight layer for the resulting concentrations in the peat. The study in this chapter will study how cracks in a continuous clay layer would affect the concentrations in the peat. The study involves simulations with a continuous (no cracks) clay layer, and with a crack at three different positions.

5.1 Model setup

5.1.1. Common features among simulations

The model setup was similar to the model in Section 4, but there were some important changes (Figure 5-1). There was a general flow of water along the model also here. However the model slope was only 0.1%. Constant head was applied at the sides and the bottom of the flow domain. The heads were in hydrostatic equilibrium at each side. The head at the left side represented an overpressure of 0.5 m, i.e. the pressure head was 0.5 m above the surface, whereas the pressure head at the right side was at the surface. The bottom head then decreased linearly from the left side to the right, i.e. slightly more than the slope of the model (which dropped 0.3 m from left to right).

Instead of a constant head at the surface of the central part of the domain, representing the peatland, a constant inflow rate was used as surface border condition at the central area of the peatland. However, the surface conditions for the outer parts of the peatland were chosen to consist of seep zones, i.e. zones without (downward) recharge but allowing (upward) discharge when pressure is above zero. The recharge at the top of the central peatland was chosen to represent an average recharge rate of 1 mm day^{-1}. This is slightly higher than the Forsmark and Simpevarp areas normal yearly average net recharge calculated as precipitation-evapotranspiration /SMHI 1995/.

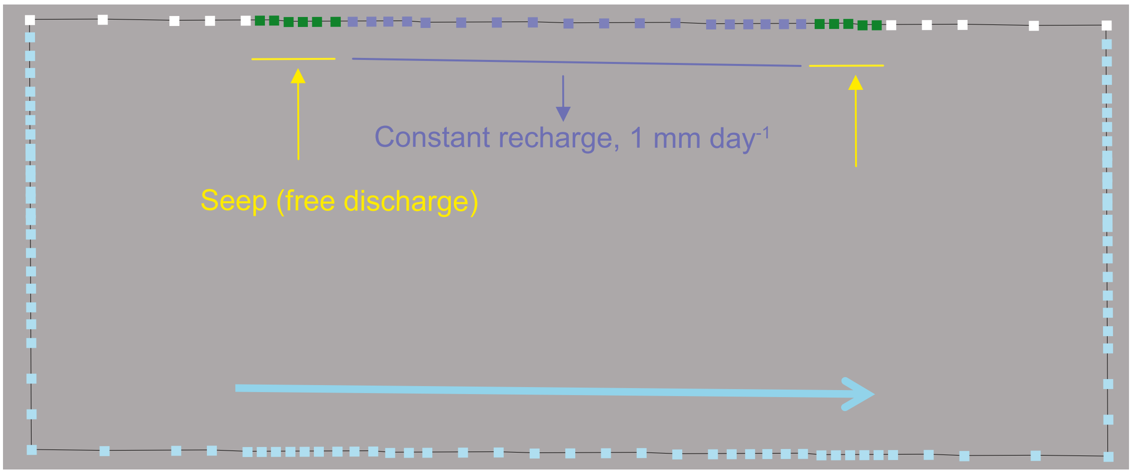

Figure 5-1. *Border conditions for the model setup for studying the effects of cracks in clay layer. The length of the model domain is 300 m and depth is 12 m. Light blue border marks denote constant head borders. White border marks denote a closed (no flux) border. The arrow denotes the major water flow direction caused by a linear decrease in the hydraulic head of totally 0.8 m from the left to the right border of the model.*

The correct number for a peatland without a surface lateral inflow is hard to know (and it varies among different surface covers /Kellner 2003/) but it probably lies between 0.5 and 1 mm day^{-1}. The hydraulic conductivity of the peat was chosen to be $k = 10^{-6}$ m s^{-1}, except in the upper 1 m where it was set to $k = 10^{-4}$ m s^{-1}. The reason for this is that the k values in the surface layers are generally much higher, decreasing 3–4 orders of magnitude within first 0.5 m depth /Ivanov 1981/. The chosen difference is thus fairly moderate.

5.1.2. Individual simulations

The four different simulations were (Figure 5-2):

5.1. A continuous clay layer.

5.2. A crack in the clay layer at the "aquifer upstream" side.

5.3. A crack in the clay layer in the central part.

5.4. A crack in the clay layer at the "aquifer downstream" side.

5.2 Results

5.2.1. A continuous clay layer

Simulating a continuous clay layer resulted in very small fluxes within the deeper layers of the peatland. The general aquifer flow direction towards the right generated a skewed concentration distribution with higher concentration of solute 2 in the left part of the peat layers (Figure 5-3). The high-conductivity layer in the upper peat caused the major part of the surface inflow water to flow more or less horizontally in this layer towards the seepage areas. The flow velocities in the deeper parts generated a Peclet number of the order of 0.1, which implies that diffusion plays an important role in solute transport.

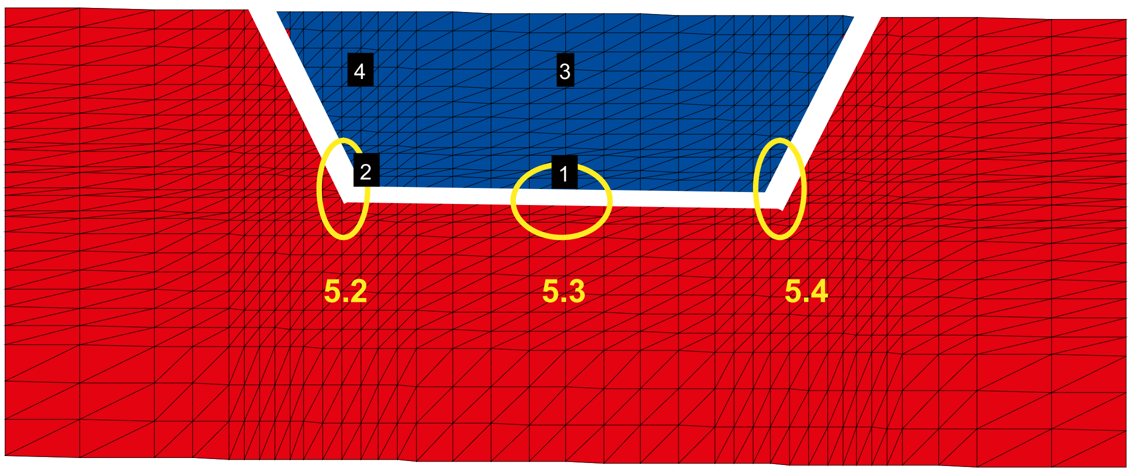

Figure 5-2. *Schematic figure of the model. The clay layer (white) separate the mineral soil (red) from the peat (blue). The numbered black marks denote four observation points where temporal variation of solute concentrations were monitored. The four different simulations were made with a continuous clay layer – simulation 5.1, a crack in the clay layer at the "aquifer upstream" side (located as marked with yellow in the figure) – simulation 5.2, a crack in the clay layer in the central part – simulation 5.3, and a crack in the clay layer at the "aquifer downstream" side – simulation 5.4.*

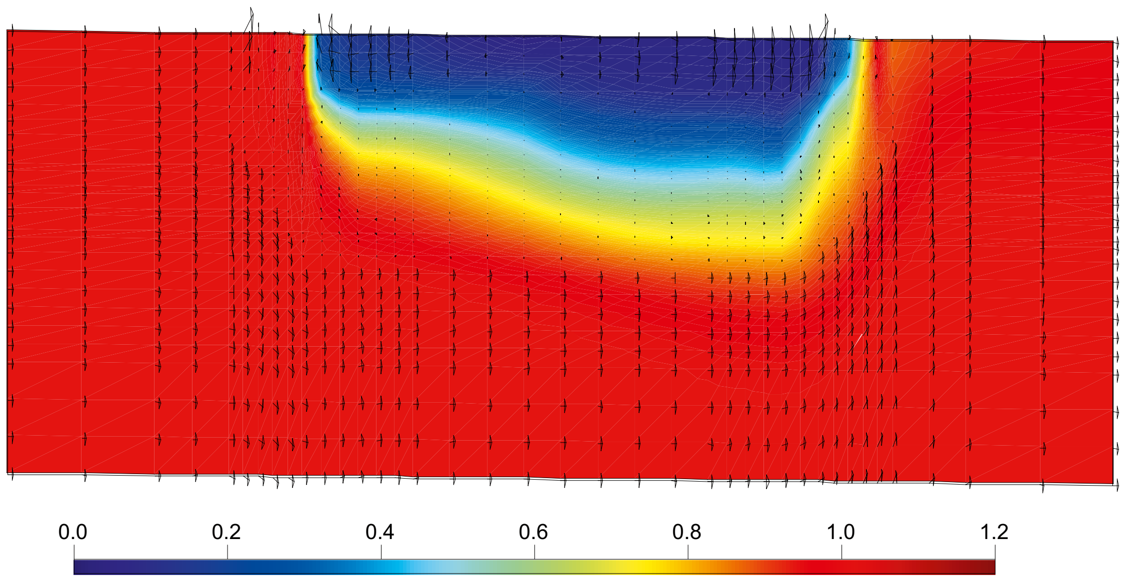

Figure 5-3. *Velocity arrows and concentration distribution of solute 2 for simulation 5.1, which has a continuous clay layer with a constant inflow at the peat surface. The spectrum bar denotes the concentration of solute 2 in µM.*

5.2.2 A crack at the upstream side

A crack in the clay layer at the left part of the peatland bottom created a shortcut effect between the higher hydraulic head in the mineral soil and the seepage zone at the surface with vertical flow velocities of up to the order of cm day^{-1}. This affected the concentrations of solute 2 at the left border and lower left part of the peat layers, whereas the right-hand side of the peat layers was not influenced notably by this. Even if the flow was slow in the deep layers, the prevalent directions were outwards from the centre parts. This restricted further effects in the deeper layers (Figure 5-4).

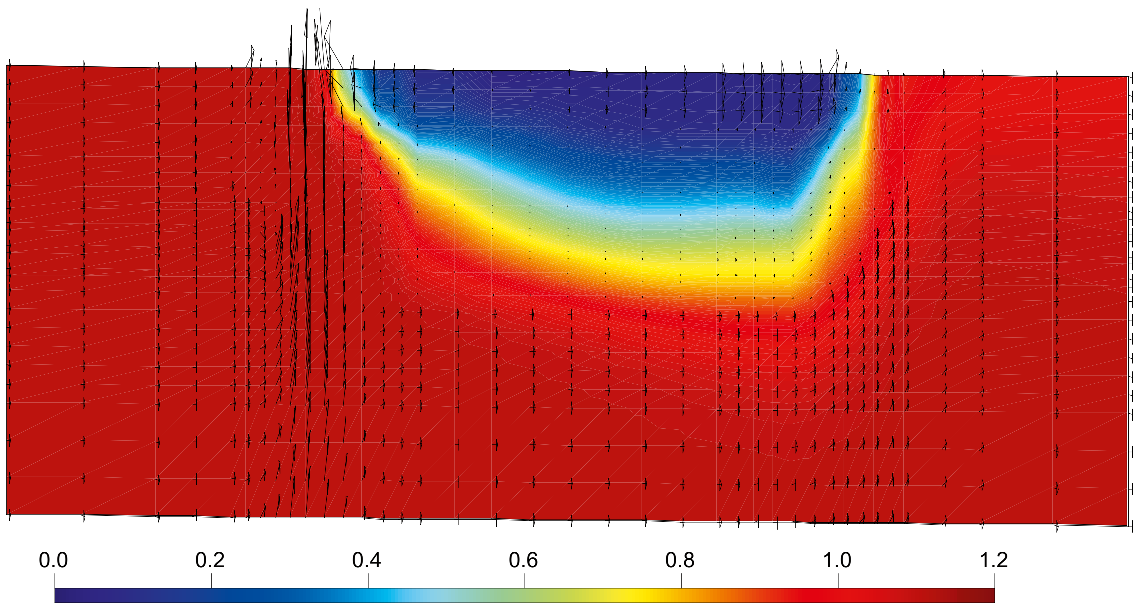

Figure 5-4. *Velocity arrows and concentration distribution of solute 2 for the simulation 5.2, which has a clay layer with a crack at the lower left corner. The mineral soil aquifer has a general flow from left to right while the peat surface has a constant downward inflow. The spectrum bar denotes the concentration of solute 2 in µM.*

5.2.3 A crack in the central part

Introduction of a crack in the clay layer in the central part caused a very small but still significant upward-directed flow. Since the velocities were very small in the centre part, even this small change caused a substantial increase in the concentration distribution (Figure 5-5).

5.2.4. A crack at the downstream side

Similarly to simulation 5.2, the crack in the clay layer created a shortcut to the seepage area on the right side. The hydraulic head gradient was smaller on the right side than on the left side. Hence, the resulting upward flow was smaller, but still up to 1 cm day^{-1}. An increase of solute 2 became evident only in the outer right parts, while the prevailing flow in the peat could keep low concentrations in the central parts (Figure 5-6).

5.2.5 Resulting solute contents

Figure 5-7 shows, besides the temporal variation at each observation point, the difference in distribution of solute 2 among the simulations. Some interesting findings are: (i) the concentration in simulation 5.3 is not only higher in the central parts, where the crack is located, but also in the upper left, (ii) the concentration in simulation 5.2 is clearly higher in the areas that are close to the crack but the concentration in the central parts is slightly lower than for the other simulations, and (iii) the crack to the right in simulation 5.4 has only an apparent effect locally, whereas the concentrations in other parts of the peatland were similar to simulation 5.1 (practically identical in Figure 5-7).

Total contents in the organic layers are presented in Table 5-1. The total contents reflect the distributions of velocities and concentrations visualized in the figures. A crack in the central part caused a substantially higher content of solute 2 than in the other simulations, whereas the amount of solute 1 did not increase much, in contrast to the simulations with cracks on the sides where the high flow velocities caused considerably higher contents of accumulated solute 1. These high inflow velocities did not have much influence on the conservative solute 2, as this was flowing through the border areas without spreading much laterally or accumulating.

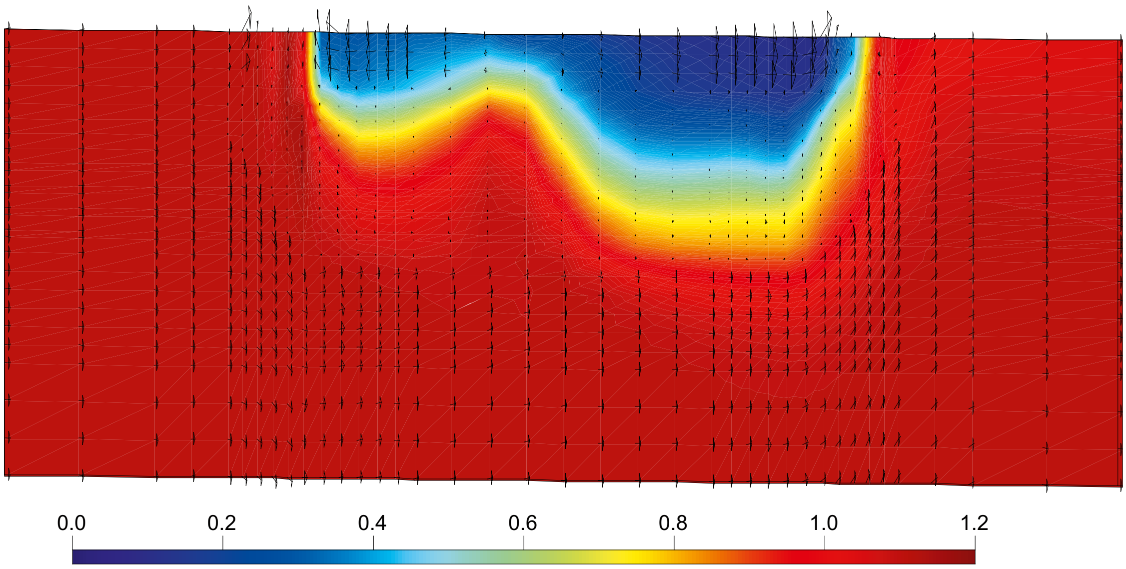

Figure 5-5. *Velocity arrows and concentration distribution of solute 2 for the simulation 5.3, which has a clay layer with a crack in the central part of the peatland. The mineral soil aquifer has a general flow from left to right while the peat surface has a constant downward inflow. The spectrum bar denotes the concentration of solute 2 in µM.*

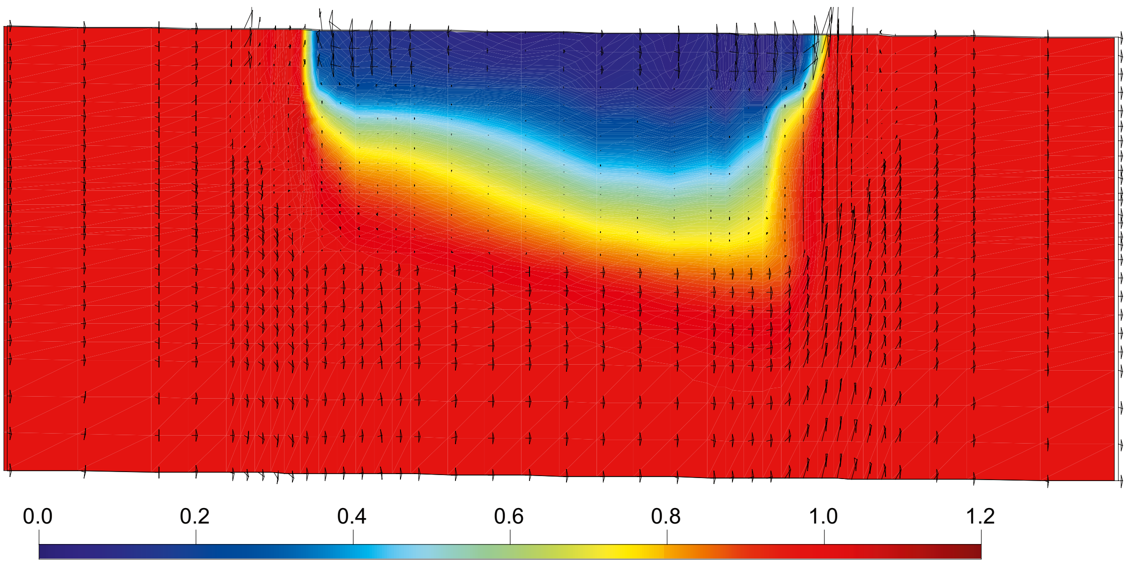

Figure 5-6. Velocity arrows and concentration distribution of solute 2 for the simulation 5.4 of a clay layer with a crack at the lower right corner. The mineral soil aquifer has a general flow from left to right while the peat surface has a constant downward inflow. The spectrum bar denotes the concentration of solute 2 in µM.

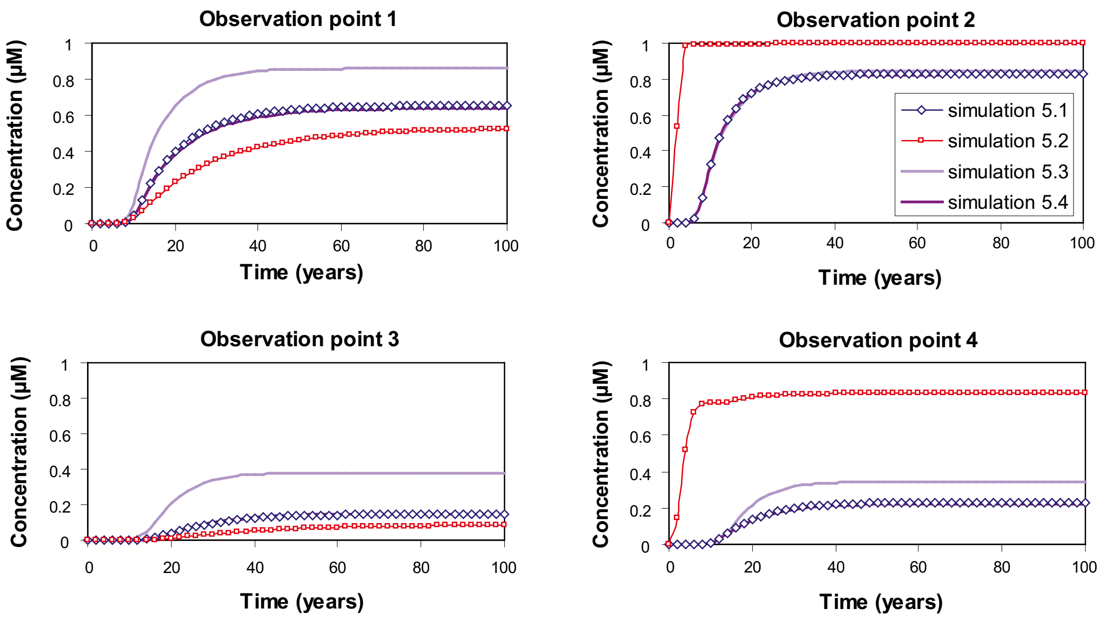

Figure 5-7. Temporal variation of solute 2 at observation points 1–4 for simulations 5.1–5.4. Locations of observation points are given in Figure 5-2.

Table 5-1. Total (and dissolved within parenthesis) amounts of solute 1 (mmoles) within model organic layers and total (= dissolved) amounts of solute 2 (mmoles) within model organic layers after 100 years.

	Simulation 5.1	Simulation 5.2	Simulation 5.3	Simulation 5.4
Solute 1	382 (0.28)	1.13×10^4 (5.05)	571 (3.3)	1,650 (1.1)
Solute 2	121.6	128.3	161.6	129.1

5.3 Discussion and conclusions

Presence of cracks in clay layers can substantially influence the contents and distributions of solutes in the peat. However, the effects will depend on the local hydraulic-head situation, flow paths in the peat and also on the character of the solute. The accumulation of an adsorptive type of solute, here exemplified by solute 1, will to large extent depend on the inflow rate, i.e. the water velocity, whereas the resulting concentrations of a conservative type of solute, like solute 2, will depend more on the prevalent directions of flow within the peat layers.

The more realistic parameterisation with a highly-permeable surface layer generated a large flow through this layer from the central part towards the borders of the peatland. The vertical flow direction was downwards except at the borders where it turned upwards in the discharge zones. This flow pattern generated a very low content of solutes in the upper part of the peatland, except at the borders.

6 Effects of anisotropy and heterogeneity

In previous chapters, it has been shown that the flow pattern in the peat is largely determined by the hydraulic conductivity and that presence of a tight layer below the peat is of significant importance for transport of solutes. Presence of tight or more permeable layers in the peat may be of similar importance for the flow pattern. This chapter presents a study of the influence of anisotropy in hydraulic conductivity within the peat and of the effect of heterogeneity.

6.1 Presence of tight peat layers

6.1.1 Description of simulations

First a study was made with tight ($k = 10^{-8}$ m s^{-1}) peat layers in an otherwise permeable ($k = 10^{-5}$ m s^{-1}) peat in a setting without clay layer. The locations of the tight layers are shown in Figure 6-1. The model setup for these simulations (6.1 and 6.2) was similar to simulation 4.9, i.e. an aquifer slope of 1% and a hydraulic-head mound at the centre of the peatland dropping off towards the sides of the peatland. The results of these simulations are only described qualitatively.

6.1.2 Results

Simulation 6.1. The resulting flow pattern and distribution of solute 2 are shown in Figure 6-2a. The upper tight peat layer had an effect of isolating the upper layer from the other layers underneath in a similar way as a bottom clay layer. Parts of the surface layer showed fairly high water velocities (> 1 cm day^{-1}). The flow above the tight layer became largely horizontal, probably because the highly-permeable surface layer was too thin to create a well-defined recharge and discharge areas. There was a part of the surface layer that had very low flow velocities, because of the counteracting local hydraulic head mound decreasing towards the left and the general model sloping towards the right. In this area, the low velocities allowed diffusive transport to cause higher concentrations than in other parts of the surface layer.

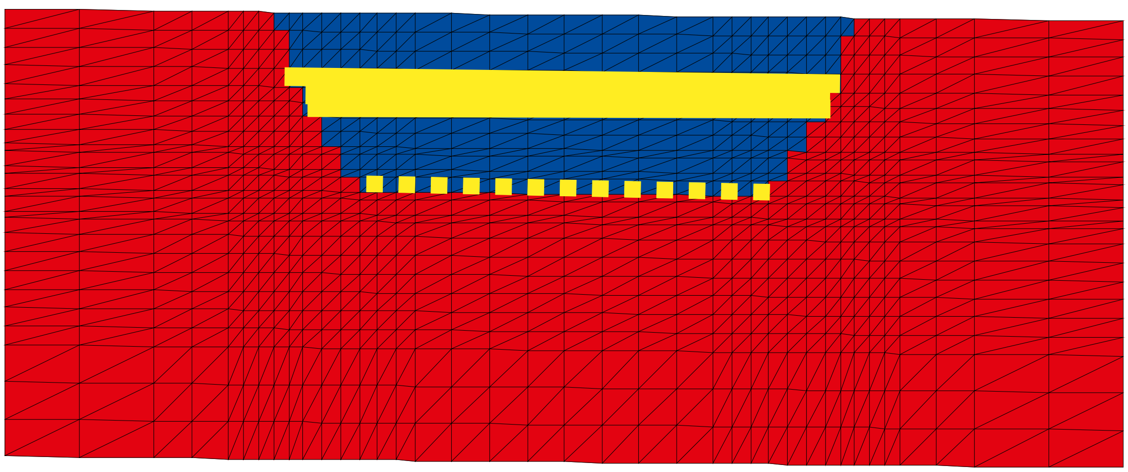

Figure 6-1. *Model setup for simulation 6.1 and 6.2. The slope and border conditions are identical to simulation 4.8. Red denotes the basic aquifer, $k = 10^{-4}$ m s^{-1}, blue denotes the base peat with $k = 10^{-5}$ m s^{-1}, the solid yellow area denotes the position of a peat layer with $k = 10^{-8}$ m s^{-1}, and the hatched yellow area a second peat layer (only in simulation 6.2) with $k = 10^{-8}$ m s^{-1}.*

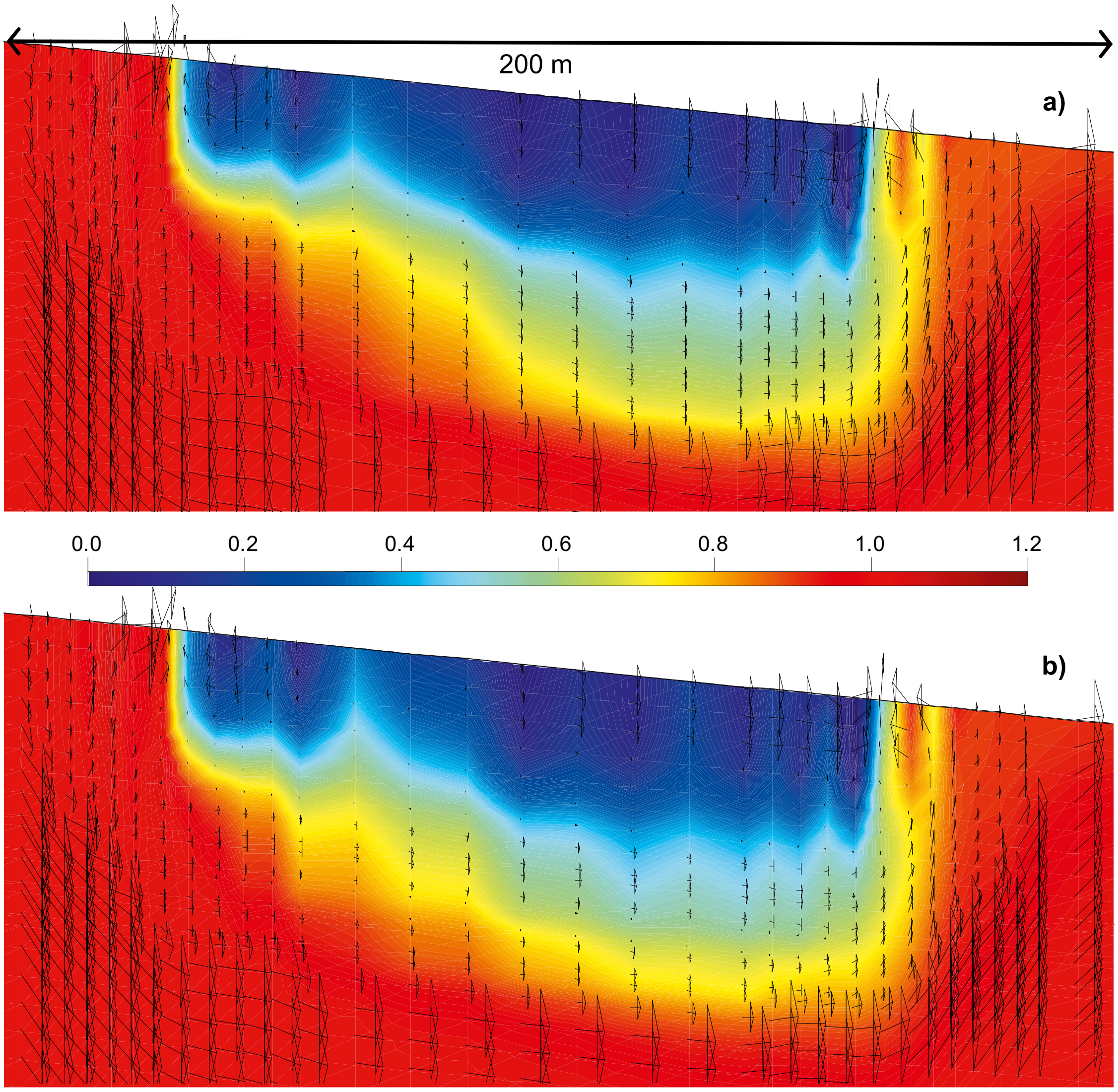

***Figure 6-2.** Velocity arrows and equilibrium concentrations of solute 2 in simulation 6.1 (a) and 6.2 (b). The spectrum bar denotes the concentration of solute 2 in µM.*

In the more permeable soil below the tight layer, the concentration increased quickly on the left side, whereas this sharp escalation declined towards the right. At the right end, the border line between the tight layer and the underlying layer could not be seen by looking at the concentration of solute 2, although it was distinctly described by the velocity arrows. It appears that the convective flow was not large enough to dominate over the dispersion/diffusion processes in the lower layers of the right part of the peatland. This is mainly because the horizontal distance is two orders of magnitude larger than the vertical distance.

Simulation 6.2. The effect of the lower layer was not so evident in this study, although a relatively sharp change in concentrations occurred over this layer. As it restricted vertical exchange, it restricted the transport of solute 2 into the next layer to some extent but not visibly for the right-side parts (Figure 6-2b).

6.1.3 Conclusion

Presence of a tight layer acts as an isolation towards the water on the other side of the layer. Similarly to a clay layer, a tight peat layer may act as a barrier and close off convective flows effectively while the importance of diffusive flow increases compared to a more permeable soil. The importance of such a layer gets reduced when flows are slow and gradients small.

6.2 Presence of highly-permeable peat layers and anisotropic peat

6.2.1 Model descriptions

Two simulations were done to study the effect of highly permeable layers. The model setup was similar to the models in Section 5, with the the peat consisting of one highly-permeable surface layer with k = 10^{-4} m s^{-1}, and one deeper less permeable layer, overlying a tight clay layer. In addition, a 0.7 m thick layer with k = 10^{-3} m s^{-1} was applied at the depth of 4 m. This heterogeneous setup was run with

- a crack in the lower left hand corner of the clay layer (simulation 6.5), resembling simulation 5.2,
- a crack in the central part of the clay layer (simulation 6.6), resembling simulation 5.3.

Two simulations were also done to study the effect of anisotropy. The setup was similar to the simulations in Section 5. Instead of applying k = 10^{-6} m s^{-1} in the lower peat layer, a horizontal k = 10^{-5} m s^{-1} and a vertical k = 10^{-7} m s^{-1} were applied, resembling a realistic anisotropy /Chason and Siegel 1986/. This anisotropic setup was run with

- a crack in the lower left hand corner of the clay layer (simulation 6.3) , resembling simulation 5.2,
- a crack in the central part of the clay layer (simulation 6.4), resembling simulation 5.3.

Simulations 6.3–6.6 were compared with homogeneous, isotropic soils, (simulations 6.7 and 6.8), similar to simulations 5.2 and 5.3, respectively. As opposed to the simulations in Chapter 5, the constant flow (recharge) at the peatland surface was set to 0.5 mm day^{-1} for these simulations (all simulations 6.3–6.8).

6.2.2 Results

Simulations 6.4 and 6.6 (a crack in the clay at the central part). The main difference between the results of the isotropic and anisotropic peat was that the anisotropic peat restricted the vertical upwards transport of solute 2. The higher horizontal conductivity did not compensate for that by increasing the lateral transport because the upward transport could not supply such an increased sideways transport (Figure 6-3, Table 6-1).

A high-conductivity layer such as that in the heterogeneous peat in simulation 6.6 increased the lateral transport at the same time as the vertical transport from bottom did not restrict the supply in the same way as the anisotropic peat did. Consequently, the concentrations increased in the lower parts on both sides of the crack (Figure 6-3, Table 6-1). The total contents of both solutes 1 and 2 also increased slightly with a high-conductivity layer, whereas they were lower in the anisotropic-peat simulation.

Simulations 6.3, 6.5 (a crack in the clay at the left border). The anisotropy in simulation 6.3 with a crack in the clay at the left border caused lower concentrations than the control (simulation 6.7). The concentrations of solute 2 became slightly lower both in the left part and in the right part.

Table 6-1. Total (and dissolved within parenthesis) amounts of solute 1 (mmoles) within model organic layers and total (= dissolved) amounts of solute 2 (mmoles) within model organic layers after 100 years.

	Simulation 6.7	Simulation 6.3	Simulation 6.5	Simulation 6.8	Simulation 6.4	Simulation 6.6
Solute 1	1.16×10^{4} (5.06)	7.18×10^{3} (3.47)	1.11×10^{4} (4.42)	994 (0.42)	624 (0.30)	1.70×10^{3} (0.59)
Solute 2	197	195	210	251	202	263

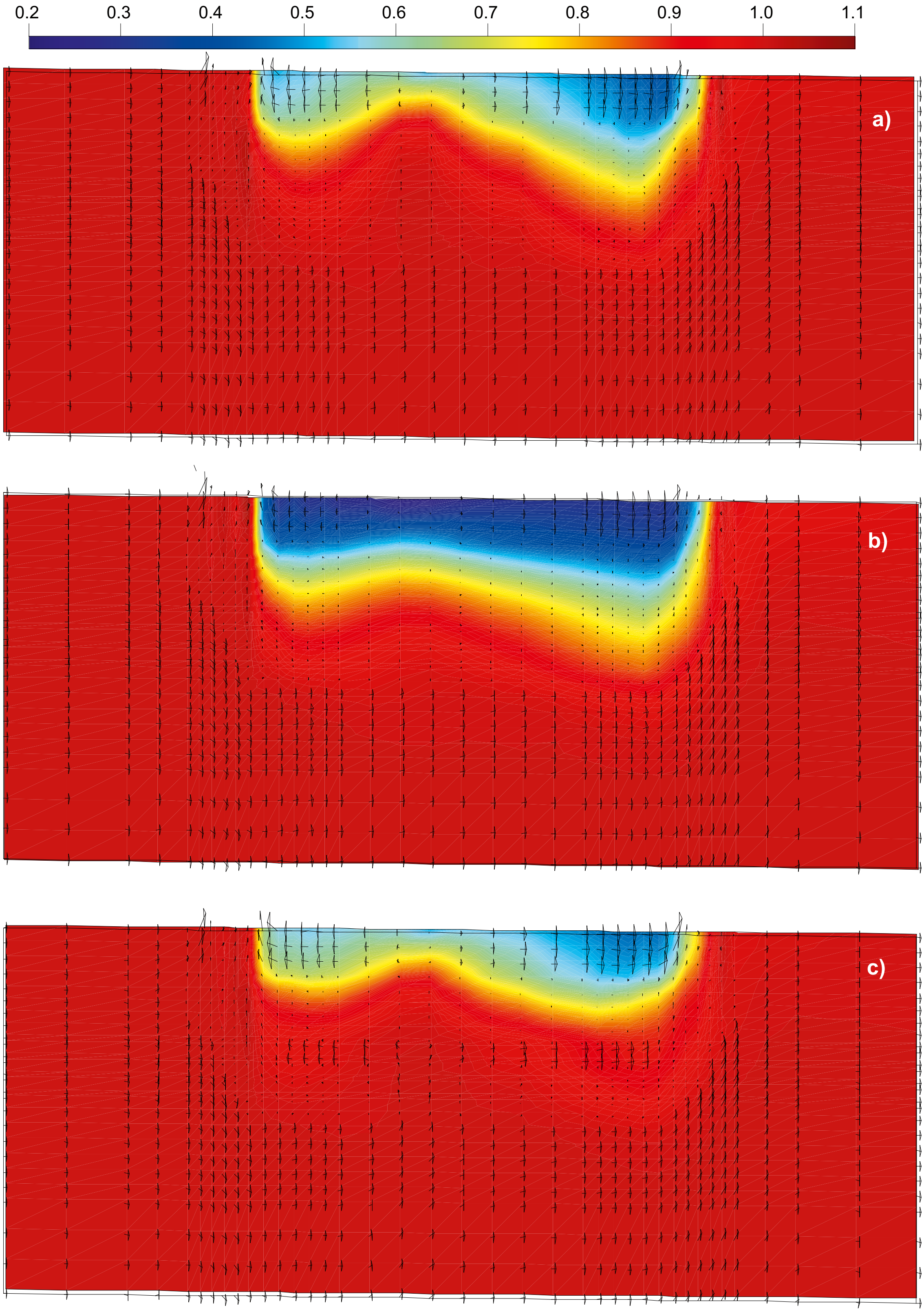

Figure 6-3. *Velocity arrows and equilibrium concentrations of solute 2 in simulation 6.8 (a) representing homogeneous isotropic peat, 6.4 (b) representing anisotropy and 6.6 (c) which includes a highly permeable layer in the peat. The spectrum bar denotes the concentration of solute 2 in µM.*

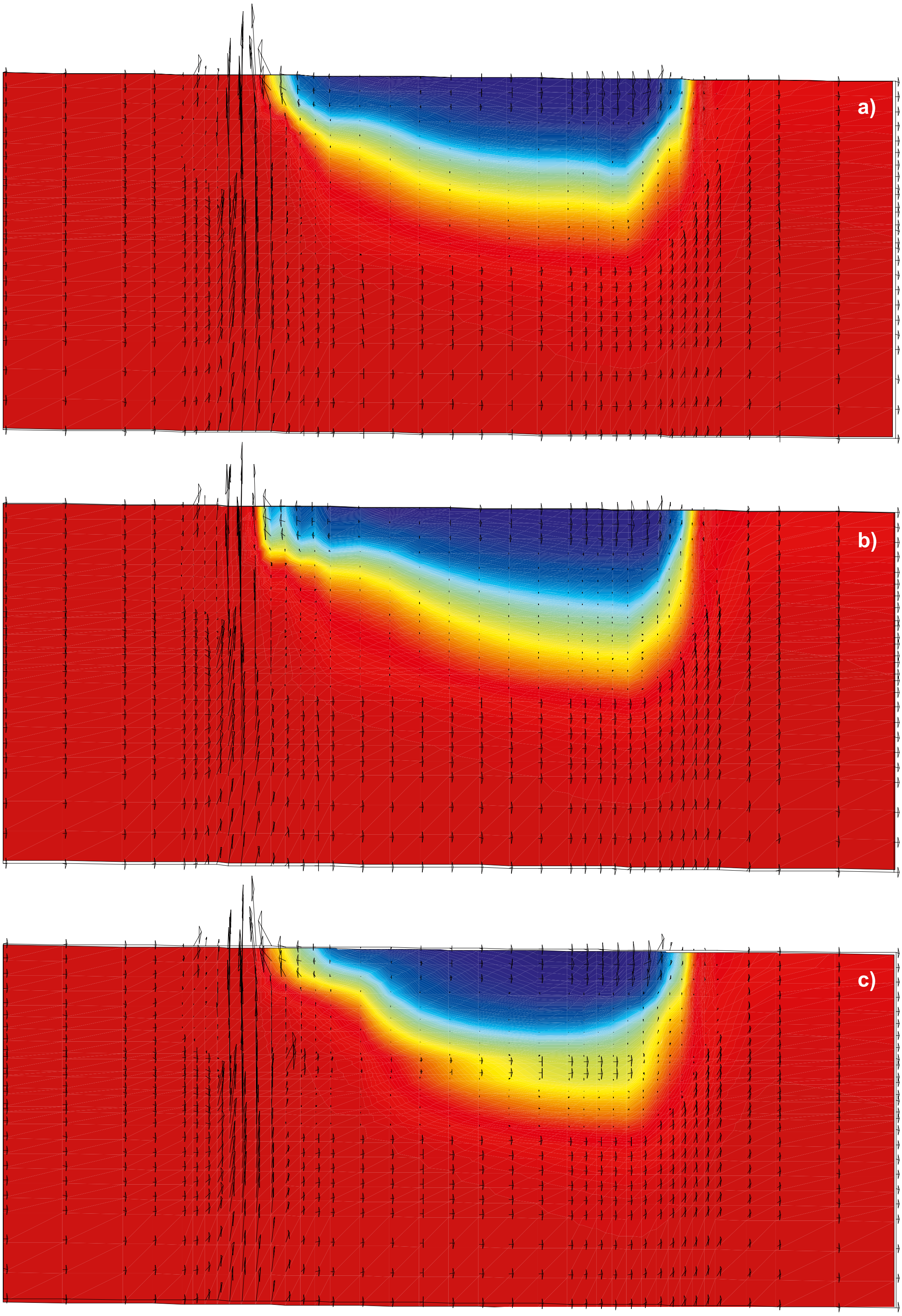

Figure 6-4. *Velocity arrows and equilibrium concentrations of solute 2 in simulation 6.7 (a) representing homogeneous peat, 6.3 (b) representing anisotropy and 6.5 (c) which includes a highly-permeable layer in the peat. The colour codes for the concentrations are the same as in Figure 6-3.*

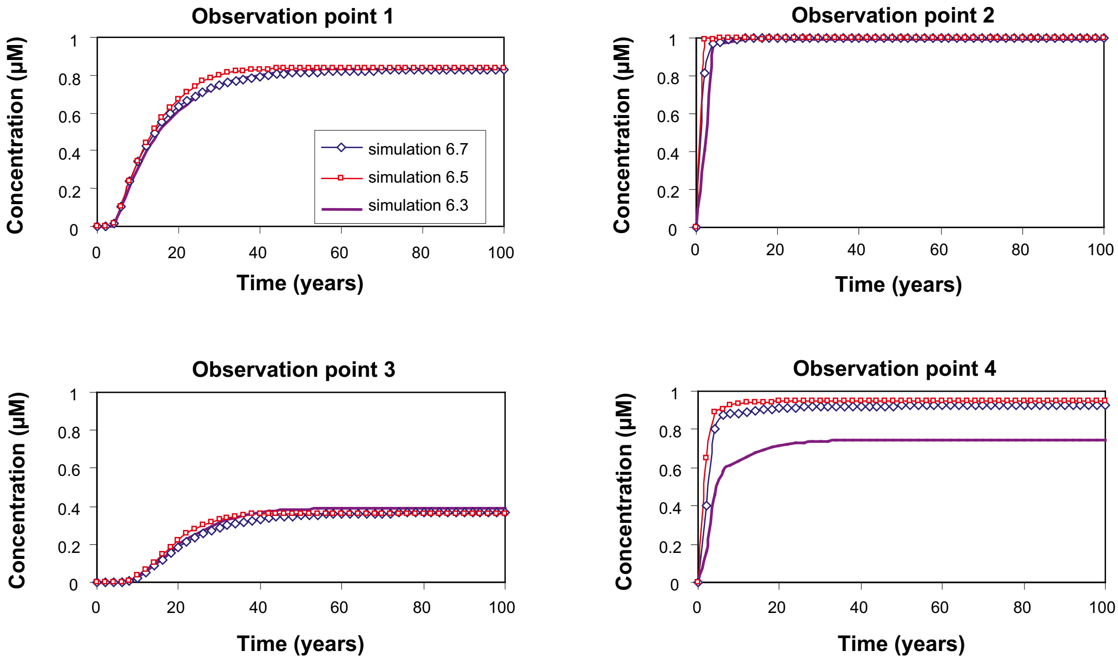

Figure 6-5. *Temporal variation of solute 2 at observation points 1–4 for simulations 6.3, 6.5 and 6.7, with a crack at the upslope side. Locations of observation points are shown in Figure 5-2.*

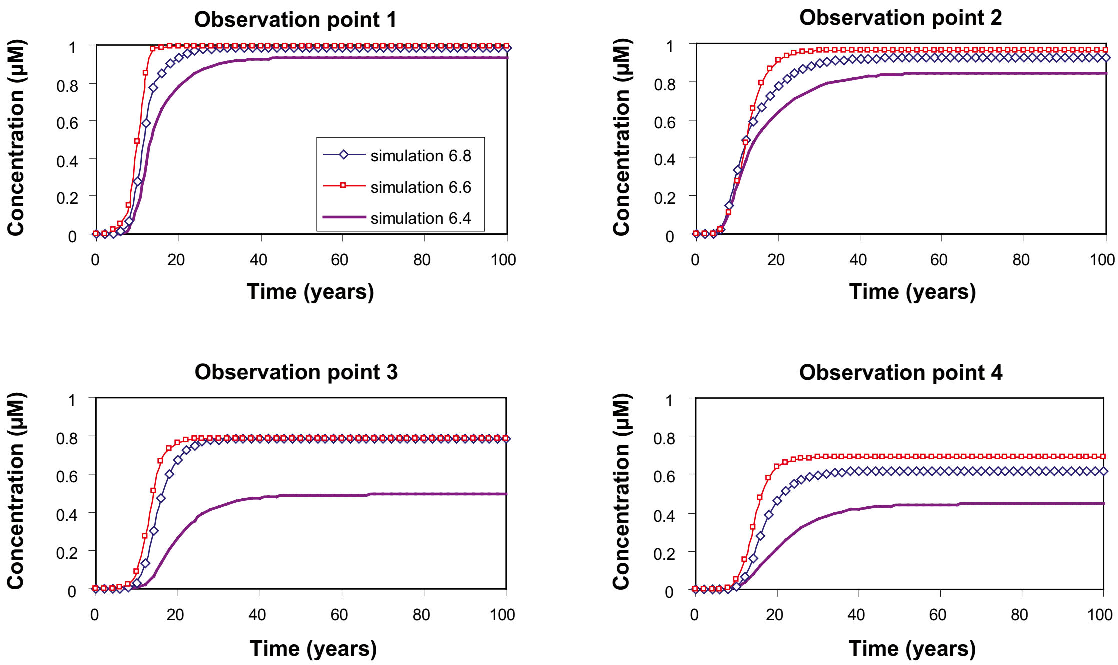

Figure 6-6. *Temporal variation of solute 2 at observation points 1–4 for simulations 6.4, 6.6 and 6.8, with a central crack. Locations of observation points are shown in Figure 5-2.*

The highly permeable layer in simulation 6.5 caused slightly higher concentrations but the concentration-enhancement effect became less on the right side. The total content of solute 2 became slightly higher in simulation 6.5 with the highly permeable layer. Also the content of solute 1 became higher in this simulation, whereas it was markedly lower in simulation 6.3 with anisotropic soil (Table 6-1).

6.2.3 Discussion and conclusions

When anisotropy or heterogeneity was included, this gave effects of consolidating or counter-acting general transport patterns, but these modifications did not change the distribution patterns radically. Partly, this can be explained by the big difference between the horizontal and vertical dimensions of the peatland. While this study has concentrated on horizontal layering with expected effects in the vertical direction, the long horizontal distances have largely evened out these effects. Another important aspect when discussing the effects is that the low velocities in the peat enhance the importance of diffusive transport. The velocity seldom exceeds 1 cm day^{-1}, and is more often on the order of mm or parts of mm per day.

7 Effects of the size of the surface recharge

The size of the recharge at the surface seems to be an important factor for the final flow pattern, and consequently for the contents and distributions of the solutes. An example is presented here by comparing the results from the simulations made in the previous section (simulations 6.7 and 6.8), with the recharge of 0.5 mm day^{-1} and corresponding simulations in Section 5 (simulations 5.2 and 5.3) with the recharge of 1 mm day^{-1}. It is clear that the smaller recharge resulted in substantially higher contents of the solutes in the peat (Table 7-1, Figure 7-1).

Table 7-1. Total (and dissolved within parenthesis) amounts of solute 1 (mmoles) within model organic layers and total (= dissolved) amounts of solute 2 (mmoles) within model organic layers after 100 years.

	Simulation 6.7	Simulation 5.2	Simulation 6.8	Simulation 5.3
Position of crack	Left	Left	Central	Central
Surface recharge	0.5 mm day^{-1}	1.0 mm day^{-1}	0.5 mm day^{-1}	1.0 mm day^{-1}
Solute 1	1.16×10^4 (5.06)	1.13×10^4 (5.05)	994 (0.42)	571 (3.3)
Solute 2	197	128.3	251	161.6

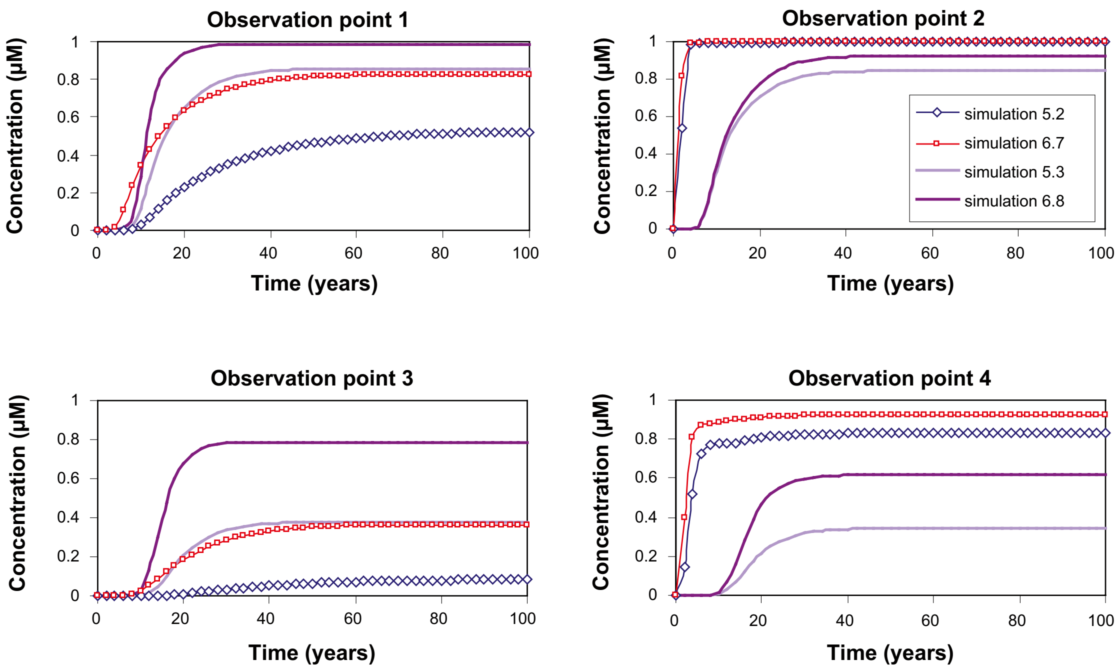

Figure 7-1. *Temporal variation of solute 2 at observation points 1–4 for simulations 5.2, 5.3, 6.7 and 6.8. Locations of observation points are shown in Figure 5-2.*

8 Effects of a seasonal variation in the recharge

The size of the recharge has been shown to be important (Chapter 7). Therefore, climatic variations should be taken into account when simulating transport during long time periods. However, one may also question if short-term average flows give a sufficiently accurate description, or if a higher resolution of temporal variations in the driving variables is needed. In this chapter, a study is presented that compares the flows and resulting concentrations from a simulation with a constant recharge and a simulation with seasonally variable recharge at the surface.

8.1 Model description

A model parameterisation similar to simulation 6.8 was chosen for simulation 8.1, but with a seasonal variation applied to the surface recharge. The values of the seasonal variation was chosen to represent a plausible variation of net recharge as the difference between precipitation and evapotranspiration based on values from /SMHI 1995/ and /Kellner 2003/. The year was divided into 6 periods, each representing 2 months. The values are given in Table 8-1 and visualized in Figure 8-1. The total average recharge was 0.52 mm day^{-1}, which was very similar to the assumed constant flux of 0.5 mm day^{-1} in simulation 6.8.

Table 8-1. Assumed fluxes of precipitation and evapotranspiration giving the net recharge that is used as the surface border inflow in simulation 8.1 (or outflow if negative). Lines presenting yearly averages of each flux and total yearly flux are also added.

Period	Precipitation (mm day^{-1})	Evapotranspiration (mm day^{-1})	Net recharge (mm day^{-1})
Jan–Feb	1.5	0.2	1.3
Mar–Apr	1	0.3	0.7
May–Jun	1.2	2	–0.8
Jul–Aug	2	3	–1
Sep–Oct	2	1	1
Nov–Dec	2	0.1	1.9
Average	1.62	1.1	0.52
Total flux per year (mm)	590	400	190

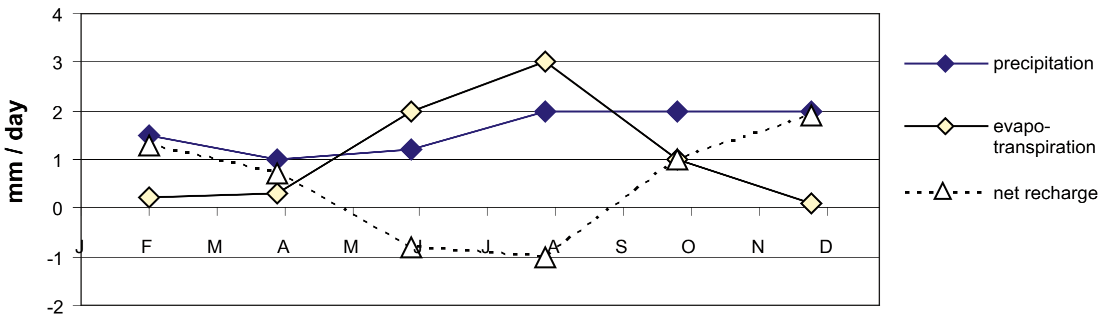

Figure 8-1. Assumed fluxes of precipitation and evapotranspiration giving the net recharge that is used as the surface border inflow in simulation 8.1 (or outflow if negative).

8.2 Results and discussion

The differences in total contents were small (Table 8-2). The varying surface recharge did result in slightly higher contents of solute 1 than the constant-rate recharge. While the total content of solute 2 was varying slightly during the seasons, between 218 and 230 mmoles (Table 8-2) , the total content was at all times slightly lower than the content of the simulation with constant recharge rate. The slightly higher contents of solute 1 can be explained by the effect of a seasonal upward flow during the summer months, which enhances the transport into the deep peat; since the adsorption is very high, this is not washed out again in the seasons of downwards flow.

It is harder to find an explanation for the slightly lower total content of solute 2. One explanation could probably be found in the fact that most of the surface recharge flows through the zone of higher hydraulic conductivity at the surface. The higher recharge rates during winter time seem to wash out much of the solute that entered the upper layers during the summer, and this effect is so strong that the total average concentration also becomes smaller than if just an average recharge flux rate is used (Figure 8-2).

The maximum concentration at the surface (0.6 µM) was reached in August, when the value was similar to the constant-rate highest surface concentration, while the highest concentrations in December and April were 0.4 µM (similar to the minimum surface concentration in the constant-rate simulation). The difference between the total contents at a varying flux and an averaged content may seem small, but the different distributions may be of importance if, for example, higher concentrations occur during the summer season when the plants are active.

Table 8-2. Total (and dissolved within parenthesis) amounts of solute 1 (mmoles) and total (= dissolved) amounts of solute 2 (mmoles) within model organic layers after 100 years for 2 different simulations, one with seasonally varying surface recharge and one with constant surface recharge.

	Simulation 8.1 Varying, 1 April	Simulation 8.1 Varying, 1 August	Simulation 8.1 Varying, 1 December	Simulation 6.8 Constant
Solute 1	1,014 (0.43)	1,024 (0.43)	1,028 (0.43)	994 (0.42)
Solute 2	218	230	221	251

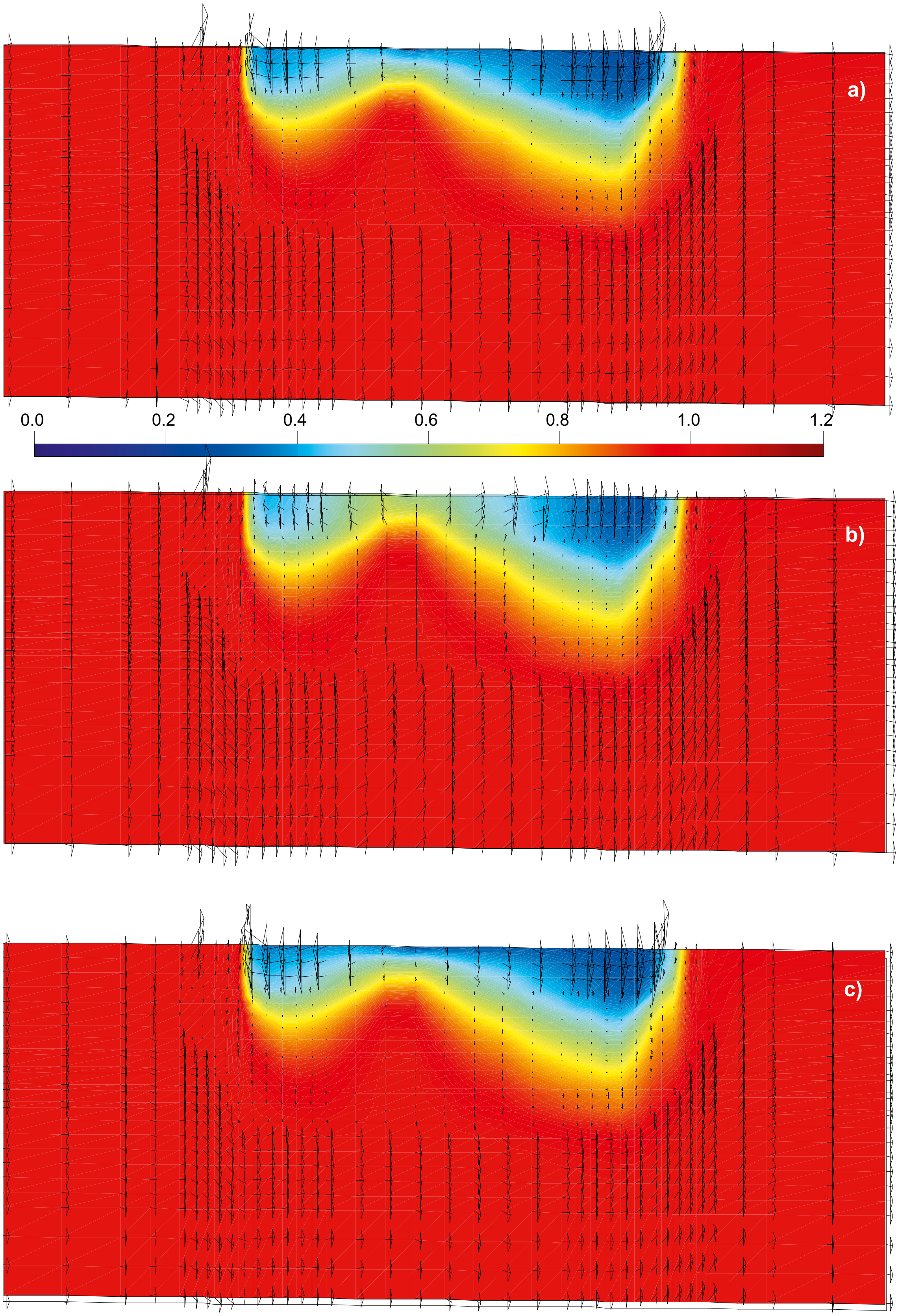

Figure 8-2. *Velocity arrows and concentrations of solute 2 in simulation 8.1 (a) on April 1, (b) on August 1 and (c) on December 1. The spectrum bar denotes the concentration of solute 2 in µM.*

9 Summarizing conclusions and discussion

9.1 Conclusions from the simulations

When modelling the flow through peatlands, the most important factor to consider is if there is any layer(s) with low hydraulic conductivity. The importance of flow direction (and hydraulic head gradient) decreases with decreasing hydraulic conductivity. This occurs as the convective flux is slowed down and the transport is taken over by the diffusive flux. The importance of a low-permeable layer increases when other layers are highly permeable. Presence of cracks in such tight layers can increase the transport of solutes into the peat. The highest inflow rates are reached when such cracks occur in discharge areas with strong upward gradients. However these areas are often also discharge areas for the flow from the peatland itself, which can counteract the distribution of the solute into the peat. On the other hand, a conservative solute can spread efficiently in a crack at low-flow (small gradient) locations if the net flow direction is towards the peatland.

One tight layer in the peat has a large importance for the flow pattern (in the same way as a clay layer) while a second tight layer influences less. Highly permeable layers as well as presence of anisotropy caused clear although not great effects on the contents of solutes. Presence of a highly permeable horizontal layer increased the lateral flow clearly, but whether solute concentrations increase due to this depends on where the solute source is located. An anisotropic peat in these simulations generally caused a smaller transport of solutes into the peatland.

Finally, the border conditions that determine the directions and sizes of fluxes are crucial for the resulting distributions. High flow rates, created by steep hydraulic-head gradients and permeable soils, generate clear differences between areas of inflow and outflow. When the flow rates are smaller, the importance of diffusion processes increases and the differences between areas of inflow and outflow get smaller. The hydraulic gradients are generally small in peatlands and a change in the size of the surface recharge (precipitation-evapotranspiration) can change the hydraulic head pattern and flow paths such that the distribution of solutes gets altered substantially. This has also the implication that seasonal shifts in the recharge may cause a seasonal variation in the distribution of a soluble compound. However, modelling seasonal variation in the surface recharge in this study produced only very small changes compared to model results using average fluxes.

On the other hand, stronger effects could occur because of long-term shifts in climate. Such variations may create alternating periods of inflow and outflow from the underlying aquifer, and the relationships between time and rates in each direction determine the resulting distribution of a conservative solute. The conditions are somewhat different for the content of an adsorptive solute, which would accumulate at the contact zone with the source, because much depends on the time and rate of inflow from the solute source. A constant, very small flux would yield smaller contents than an identical net flux that was alternating with somewhat greater up- and downward fluxes.

9.2 Comparison with 3D simulations of the Forsmark area

The simulated peatlands in this study are simplified with hypothetical flow settings, and the results need to be interpreted with great care. In connection with this work a study was made with a 3D model describing the water flow in three different peatlands that were supposed to develop by terrestrialisation, i.e. by filling of three current lakes (Bolundsfjärden, Eckarfjärden and Puttan) in the Forsmark area /Vikström and Gustafsson 2006/. The model peatlands in their study were parameterised as the current lake sediments covered by peat layers up to the level of current lake surfaces. Their model was then run with conditions set by current normal climate data and regional groundwater flows, adjusted for changes in hydraulic head by the land uplift and the addition of peat in the lakes. Here, we compare and discuss the findings in the present study and those of /Vikström and Gustafsson 2006/.

/Vikström and Gustafsson 2006/ compared how different peat hydraulic properties and different peatland vegetation types influenced the net flows to and from an upper and a lower zone in the simulated peatland at Lake Bolundsfjärden. A vegetation cover yielding greater evapotranspiration resulted in less surface runoff, more groundwater boundary inflow and less boundary outflow. This means that one could expect higher concentrations of solutes if the source was in the deep groundwater. A vegetation cover yielding less evapotranspiration resulted consequently in higher water table levels, more surface runoff and more groundwater-boundary outflow, which means that lower concentrations of solutes from deeper layers could be expected.

Three different peat hydraulic conditions were also compared, with values of the hydraulic conductivity ranging between 10^{-8} and 10^{-4} m s^{-1}. The peat layers were homogeneous and isotropic. The *sapric* peat ($k = 10^{-8}$ m s^{-1}) resulted in smaller vertical flow than the other two peat types, *hemic* peat ($k = 10^{-6}$ m s^{-1}) and *fibric* peat ($k = 10^{-4}$ m s^{-1}), whereas the difference between these latter types was small. Thus, the groundwater exchange with deeper layers was smaller for the *sapric* peat, while the overland fluxes were greater. This is consistent with the results in this study although the small difference between the *hemic* and *fibric* peats may appear confusing.

However, the bottom sediments in the study of /Vikström and Gustafsson 2006/ were largely consisting of gyttja, which was assumed to have the same hydraulic properties as clay. Thus, the bottom gyttja sediments were restricting the exchange between the peat and the deeper layers rather than the *hemic* and the *fibric* peats themselves. /Vikström and Gustafsson 2006/ did not discuss any spatial differences within the peatlands in connection with these comparisons of hydraulic properties and land surface cover and no simulation of solute transports was included in this part of their study. Therefore, the effects found in this report of flow cells forming in permeable peat above a tighter layer cannot be confirmed.

The presence of a tight bottom sediment turned out to be very important for the vertical groundwater flow for the simulated peatland at Eckarfjärden, where significant fluxes only occurred along the peripheral borders of the peatland (the areas in the current lake that have no or a very thin clay layer). These areas acted as recharge and discharge areas depending on the direction of the hydraulic gradient, but generally the areas close to the outlet were acting as constant discharge areas while areas more distant from the outlet acted as recharge areas during wet periods and as discharge areas during dry periods. Puttan, on the other hand, had less diversified flows and almost the whole peatland acted as a discharge area, although the greatest fluxes occurred close to the borders. Also the flows at the peatland of Bolundsfjärden were clearly restricted in the areas where substantial gyttja layers covered the lake sediments. In the areas with thinner gyttja layers at the inlet and outlet of Bolundsfjärden, strong recharge (inlet) and discharge (outlet) areas formed, as an effect of the large difference in water level between the inlet and outlet areas

If we compare the simulations in Chapters 5–8 with the simulations of Eckarfjärden and Puttan, the importance of a tight layer is evident both in this study and in the study by /Vikström and Gustafsson 2006/. Presence of a low-permeable peat layer, a gyttja layer or a clay layer slows down the water movement, and thus also the transports of solutes. However, concerning the direction of flow, it is more determined by climatic input and where the peatland is located in the local topography and geology. The resulting concentrations will depend on the mixing ratio of water with sources from above and below, i.e. in a recharge area high-permeable sediments will cause lower concentrations than a low-permeable sediment if the source of the solute is in the deep groundwater.

Consequently, in a discharge area, a high-permeable sediment will cause higher concentrations than a low-permeable sediment. Flows of importance occur in areas with less thick clay sediments. Consequently the importance of the water-table level is great in these areas. For example, at Eckarfjärden the flow direction in some parts is changing from strong discharge (upwards) in September to strong recharge (downwards) in December. The concentration in the soil layers was determined by the mixing ratio of the water from different origins.

/Vikström and Gustafsson 2006/ also found that besides the presence of tight layers, the most important factor for the groundwater flow was the size and the direction of the hydraulic head gradient. The length scale was larger in the simulations of /Vikström and Gustafsson 2006/ than in this study. While horizontal flows could be significant in this study, the vertical flows were much greater than the horizontal flows in their study. The horizontal flow velocity was very low, in the order of 10^{-6} mm/day compared to vertical flows of normally 0.01–1 mm day^{-1}, i.e. horizontal flows were about six orders of magnitude smaller than the vertical flows. Thus, the distributions of pollutants coming from bottom layer sources depended on the vertical flows, i.e. on the vertical hydraulic head gradients and the hydraulic conductivity. Consequently, the water levels in the simulated peatlands became a very important factor because the relationship between the hydraulic head at the surface and in the underlying layers determines this gradient.

This leads to a high sensitivity to the water levels at the peatland surfaces, which means that the parameterisation of the water level at the peatland surface becomes important. In the model study of /Vikström and Gustafsson 2006/, the peatland surfaces were assumed to be flat but the water table developed a slope towards the outlet in order to enable surface discharge from the peatlands. The slope of the water table was determined by the supply of water to the peatland and the roughness of the surface (given as a Manning number, M). The Manning number for the peat surface was set to M = 3 to represent a highly vegetated surface, while water courses crossing the peatlands were assigned a Manning number of M = 10. These numbers are very low, compared to natural rivers for instance, representing highly flow-resistant surfaces.

Since such rough surfaces require steep horizontal gradients in order to evacuate a certain flow the models created very high water levels rising upstreams from the outlet along the peatland surfaces. This occurred especially in the area of current Lake Bolundsfjärden, which has a catchment bigger than the others and a significant stream inflow. The stream inflow caused a high ponding (> 1 m) on the peatland in that part; this type of ponding was much larger than one would expect in a natural peatland. The model should probably have benefited from a wider stream bed with higher Manning numbers through the peatland. In the two peatlands with small catchments (Puttan and Eckarfjärden) the simulated water levels were more moderate (mean levels of 0.02 m and 0.18 m at Eckarfjärden and 0.06 m and 0.11 m at Puttan in early September and in late December, respectively). The slope of the water table in those smaller peatlands was about 0.1 m per 100 m.

9.3 Should models allow ponding on peatland surfaces?

Although peatlands can be considered to have a continuously shallow water table, the depth of ponded water is seldom very large in this climate zone. Usually there is some micro-topography consisted of peat ridges and hollows with up to 40 cm amplitude (in other areas in Sweden with wetter climate, deeper water-filled hollows called pools are more common). When wet periods occur and surface water forms, this topography will restrict surface runoff and some ponds will form in the hollows. However, when the water table reaches some point there are most often lower patches that interconnect the water bodies and a "shortcut" surface runoff forms, see e.g. /Quinton and Roulet 1988/. Thus, even if the ridges restrict the surface flow, this seldom creates more than temporary patches of standing surface water in hollows. An exception is a type of peatland, occurring in Northern Sweden and Finland, with more conspicuous ridges called strings that continuously keep extensive pools of water.

Consequently, one can argue that the water depth distributions in the simulations of /Vikström and Gustafsson 2006/ were unrealistic because of the standing surface water. This was true especially in the case of the peatland at Lake Bolundsfjärden, where the surface water inflow by a stream was not efficiently drained away. This large inflow was not taking place in the smaller peatlands, and the main arguments against a parameterisation that causes standing water on these peatlands come from hydrological reasons rather than hydraulic. In other words, the simulated hydraulic head gradients were of similar sizes as the expected real gradients.

However, the slope of a real peatland surface most often is the same as the slope of the water table, as the peat thickness adapts to keep the surface moist (e.g. /Ivanov 1981/). Thus, there is often a slope through a peatland towards its surface-water outlet. With a moderate water input in this climate we could expect a slope of the order of 0.1 m per 100 m, which is identical to the slopes in the simulations discussed in Chapters 5–8 in this report and close to the resulting slopes in the simulations of the peatlands located at Eckarfjärden and Puttan /Vikström and Gustafsson 2006/. Therefore, one can consider the water-table levels of these two simulated peatlands to be realistic, given that the inflow-outflow rates are realistic.

However, even if the hydraulic heads are realistic the model sections of evapotranspiration and plant functions will not work in a proper way if the surface is waterlogged to such an extent. A continuous water body will also generate much faster horizontal transport of solutes because of wind-induced currents etc. On the other hand, the very low Manning numbers of the model by /Vikström and Gustafsson 2006/ probably restrict such lateral movements. To conclude, using low Manning numbers instead of a set slope of the surface will give opportunity for the model to develop slopes of the water table instead of pre-determined slopes, but the resulting slopes will likewise depend on the determined Manning numbers.

Another big difference is that there was no surface water inflow in this study while surface water inflow was a major source for the simulated peatlands in the study of /Vikström and Gustafsson 2006/. The 3-dimensional simulation can be seen as more realistic in this respect as it considers the hydrology for adjacent parts. The main difference with a significant surface water inflow would be that the importance of the precipitation recharge decreases. In the simulations of this study, where no surface inflows or outflows existed, the surface water table or hydraulic head developed to have its maximum in the centre of the peatland. The net precipitation water created a groundwater mound, with a height that was determined by the size of the net precipitation and the hydraulic conductivity in the surface layers.

In the simulations of /Vikström and Gustafsson 2006/, there were no indications of bog groundwater mound formation. In their simulations the lateral inflow to every peatland was significantly larger than the net precipitation. Although the sizes of the different recharge terms vary over the seasons, the size of the lateral inflow was always large enough to be the dominant inflow term in the water budget. For Puttan and Eckarfjärden, the main inflow areas were along the borders, and there was a general slope from the most remote areas towards the outlet. For Bolundsfjärden the slope of the water table was determined by the size of the inflow at the inlet.

9.4 Possibilities to improve the surface-layer descriptions

In addition to the somewhat inaccurate stream description in the simulation of the Bolundsfjärden peatland, it is possible that the water table level in the simulations of /Vikström and Gustafsson 2006/ would be distributed differently if the surface was described to have a smaller roughness, allowing the water to run off without ponding. This would then require a sloping surface with realistic hydraulic properties because hydraulic properties of the surface are important for a realistic description of the water flows.

/Ivanov 1981/ suggested that the hydraulic conductivity in the top layers of peatlands should be described in terms of transmissivity ("modulus of seepage"), where the total permeability of the surface layer is integrated through the layer by a function that depends on the level of the water table. This function is giving increasing transmissivity with increasing level of water table, often by a power function of the water table level. /Ivanov 1981/ also suggested a number of such functions for different types of peatlands.

In principle, it would be fairly easy to assign a range of such functions to a model, although this parameterisation is more suitable for analytical models than for finite-element or finite-difference methods. However, in the selection of parameters for the surface hydraulic conductivity, one has to be aware of the natural ecohydrological conditions in different types of peatlands, i.e. the water table should only be allowed to vary within a certain range typical for the simulated peatland vegetation type. For a specific climate, a specific type of peatland will have a certain slope that is adjusted to the net water recharge in order to keep the water table within a certain range typical of that peatland. Moreover, as hinted above, the real peatland is a dynamic system which complicates the parameterisation describing the distribution of hydraulic conductivity. For example, if the climate changes, the real peatland either changes its surface type (hydraulic conductivity) or develops a different topography and eventually a different slope.

9.5 Other potentially important processes

The presence of a highly permeable surface layer generates some interesting issues concerning the impact on the flow paths. The high hydraulic conductivity, which increases to practically infinity when water table reaches the surface, will readily drain away large recharge events, avoiding high hydraulic heads that would generate downward flow and thus creating a disagreement between theoretical distribution of flows and the resulting real flow paths. A special case of such disagreement is the condition that is created by the presence of soil frost in winter, which in peatlands likely is solid ice. The winter precipitation will then form surface runoff without contact with the peat /Laudon et al. 2005/. Although this issue has important implications, very little is known about the real flow paths and their possible changes in time, and there is a considerable need for more studies in this area.

Other potentially important factors are the effects of the compressibility of the peat and of biogenic peat gas that forms bubbles. The compressibility of the peat causes variations of peat volume by subsidence and swelling, even under normal seasonal variations in water table. In undisturbed peatlands, the seasonal change in surface level has been measured to be in the range of 40–100 mm /Kellner and Halldin 2002, Kellner et al. 2003/, and this phenomenon has several implications. It changes the important water table-soil surface relation, i.e. a certain water-table level that applies a certain hydraulic head at the surface can either be quickly declining or be in a relatively stable position depending on its position compared to the surface.

The volume changes themselves also create seasonal changes of hydraulic conductivity that can be several orders of magnitude in some layers /Price 2003/. Gas bubble volumes of 10% of total peat volumes have been found /Rosenberry et al. 2003/, and also seasonal variations of gas bubbles between 2 and 15% have been found in the upper metre /Kellner et al. 2005/. Such seasonal variations can further cause seasonal variations in the hydraulic conductivity by several orders of magnitude /Beckwith and Baird 2001/.

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Appendix

Description of the model and a list of used parameters

The modelling tool used in this work is HYDRUS-2D. While full documentation is given by /Šimunek et al. 1999/, information on this program can be obtained at:

http://www.mines.edu/igwmc/software/igwmcsoft/hydrus2d.htm (address valid February 2007), from which the following description is acquired.

"The HYDRUS2D program is a finite element model for simulating movement of water, heat, and multiple solutes in variably saturated media. The program numerically solves the Richards' equation for saturated-unsaturated water flow and the Fickian-based advection-dispersion equations for heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equation considers conduction as well as convection with flowing water. The solute transport equations consider advective-dispersive transport in the liquid phase, and diffusion in the gaseous phase. The transport equations also include provisions for nonlinear and/or nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions: one which is independent of other solutes, and one which provides the coupling between solutes involved in sequential first-order decay reactions.

HYDRUS2D can handle flow regions delineated by irregular boundaries. The flow region itself may be composed of non-uniform soils having an arbitrary degree of local anisotropy. Flow and transport can occur in the vertical plane, the horizontal plane, or in a three dimensional region exhibiting radial symmetry about the vertical axis. The water flow part of the model can deal with (constant or time-varying) prescribed head and flux boundaries, as well as boundaries controlled by atmospheric conditions. Soil surface boundary conditions may change during the simulation from prescribed flux to prescribed head type conditions (and vice versa). The code can also handle a seepage face boundary through which water leaves the saturated part of the flow domain, and free drainage boundary conditions. Nodal drains are represented by a simple relationship derived from analog experiments.

For solute transport the code supports both (constant and varying) prescribed concentration (Dirichlet or firsttype) and concentration flux (Cauchy or thirdtype) boundaries. The dispersion tensor includes a term reflecting the effects of molecular diffusion and tortuosity.

The governing equations are solved using a Galerkin type linear finite element method applied to a network of triangular elements. Integration in time is achieved using an implicit (backwards) finite difference scheme for both saturated and unsaturated conditions. The resulting equations are solved in an iterative fashion, by linearization and subsequent Gaussian elimination for banded matrices, a conjugate gradient method for symmetric matrices, or the ORTHOMIN method for asymmetric matrices. To minimize numerical oscillations upstream weighing is included as an option (not used here) for solving the transport equation."

In the work of this report, no water uptake by plant roots was simulated. No heat transport calculations were done. Because the model was continuously saturated at all nodes, no gas transports were simulated. Adsorption was determined by a linear relationship between adsorbed (s) and dissolved concentrations (c), governed by the adsorption coefficient (K), i.e. $s = K\,c$, with values for the different soil types as described in Table 3-1. Instantaneous adsorption was assumed.

The parameterization to follow is described using the vocabulary of the software menus and is also divided in the same way as the pre-processing submenus, titles of which are given in bold style. Full explanation of all the terms and parameter codes are given in /Rassam et al. 2004/.

Main processes:

Water flow and solute transports.

Geometry information:

The model was set in a rectangular form, elements ordered in a vertical plane as well as the flow. There were five different materials and two flow domains (organic soil domain and total model domain), for each of which the mass balance was calculated.

Time information:

Selected time units: Days.
Initial time: 0.
Final time: 36,500.
Initial time step: 0.1.
Minimum time step: 0.001.
Maximum time step: 10.
Time-variable boundary conditions (yes/no): These were only used in simulation 8.1.

Water flow – Iteration criteria:

The initial conditions were determined by the water pressure along the borders.

Water flow – Soil hydraulic model and Soil hydraulic parameters:

The soil unsaturated hydraulic conditions were determined by the concept of *van Genuchten – Mualem.* In unsaturated conditions (water pressure $h < 0$), the volumetric soil water content θ is determined by:

$\theta = \theta_r + (\theta_s – \theta_r)/(1 + (\alpha h)^n)^m$

where θ_s and θ_s denote the residual and saturated water content, respectively, while α and n are parameters expressing the air-entry pressure and pore size distribution, respectively, and m = (1–1/n). The hydraulic conductivity (k) depends on the saturated hydraulic conductivity (k_s) and the saturation S_e ($S_e = [\theta – \theta_r]/[\theta_s – \theta_r]$):

$k = k_s\, S_e^{l}\, [1–(1–S_e^{\ 1/m})^m]^2$

in which l is a parameter for pore connectivity. However, the top soil was very seldom unsaturated in the simulations presented here.

The effective porosity (volumetric part of water-conducting pores) was determined by the difference between residual water content and saturated water content. Normal peat soils have a high total porosity, typically $\theta_s = 0.8$. However, a lot of peat pore space is not contributing to water flow because of discontinuous pores. To obtain a realistic value of effective porosity the saturated water content was determined to only $\theta_s = 0.5$ for peat soils and 0.43 for mineral soils, while the residual water content was set to $\theta_r = 0.08$ for all soils. The parameters n, α and l were set to 1.56, 3.6 and 0.5, respectively, for all soils.

No hysteresis was accounted for.

The Water Flow Parameter matrix was thus as follows:

Mat	Qr	Qs	Alpha	n	Ks	l
1	0.078	0.5	3.6	1.56	variable	0.5
2	0.078	0.5	3.6	1.56	variable	0.5
3	0.078	0.43	3.6	1.56	variable	0.5
4	0.078	0.43	3.6	1.56	variable	0.5
5	0.078	0.43	3.6	1.56	8.64	0.5

Solute transport:

Time weighting scheme: Crank-Nicholson scheme.

Space weighting scheme: Galerkin Finite elements.

Mass units: mmol.

Stability criterion, given as Peclet number × Curant number: 2.0.

Transport and reaction parameters are not chosen to be depending on temperature.

A tortuosity factor according to the formulation of /Millington and Quirk 1961/ was used to adjust the molecular diffusion coefficients in the water and gas phases.

Number of solutes: 2.

Pulse duration 365,000.

Solute transport parameters:

Soil specific parameters.

Material (layer)	Bulk density	Dispersivity longitudinal	Dispersivity transverse	Fract.*	Thlmob.**
1	200	0.1	0.01	1	0
2	200	0.1	0.01	1	0
3	1,500	0.5	0.01	0	0
4	1,500	0.1	0.01	0	0
5	1,500	0.1	0.01	0	0

*Fract: Fraction of the sorption sites subject to instantaneous sorption.

**Thlmob: Immobile water content when physical nonequilibrium is simulated.

Solute specific parameters: Molecular diffusion coefficient in free water was 0.001 for both Solute 1 and Solute 2.

Reaction parameters for solute 1:

Solute transport parameters:

Material	Kd	Nu	Beta	Henry	SinkL1	SinkS1	SinkG1	SinkL1’	SinkS1’	SinkG1’
1	10	0	1	0	0	0	0	0	0	0
2	10	0	1	0	0	0	0	0	0	0
3	0	0	1	0	0	0	0	0	0	0
4	0	0	1	0	0	0	0	0	0	0
5	0	0	1	0	0	0	0	0	0	0

Material	SinkL0	SinkS0	SinkG0	Alpha
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0

Boundary conditions:

	cBnd1	cBnd2	cBnd3	cBnd4	cRoot	cWell	cBnd7	cAtm	d
1	0	1	0	0	0	0	0	0	0

Reaction parameters for solute 2:

Solute transport parameters:

Material	Kd	Nu	Beta	Henry	SinkL1	SinkS1	SinkG1	SinkL1’	SinkS1’	SinkG1’
1	0	0	1	0	0	0	0	0	0	0
2	0	0	1	0	0	0	0	0	0	0
3	0	0	1	0	0	0	0	0	0	0
4	0	0	1	0	0	0	0	0	0	0
5	0	0	1	0	0	0	0	0	0	0

Material	SinkL0	SinkS0	SinkG0	Alpha
1	0	0	0	0
2	0	0	0	0
3	0	0	0	0
4	0	0	0	0
5	0	0	0	0

Boundary conditions:

	cBnd1	cBnd2	cBnd3	cBnd4	cRoot	cWell	cBnd7	cAtm	d
1	0	1	0	0	0	0	0	0	0

Rectangular geometry:

Horizontal rectangular dimension: 300.
Vertical rectangular dimension: 12.
Slope of the base: –0.001.
Number of vertical columns: 39.
Number of horizontal columns: 26.

Space discretization:

Horizontal discretization (grey cell is denoting column number):

x-coord	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
	0	20	40	50	60	64	68	72	76	80	85	90	95	100	105	110	120	130	140	150
dz	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Horizontal discretization, continued:

x-coord	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39
	160	170	180	190	195	200	205	210	215	220	224	228	232	236	240	250	260	280	300
dz	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Vertical discretization (grey cell is denoting column number):

z-coord	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
	12	11.5	11	10.5	10	9.6	9.2	8.8	8.4	8.2	7.8	7.6	7.2	7	6.6	6.4	6	5.5	5	4.5	4	3.5	3	2	1	0