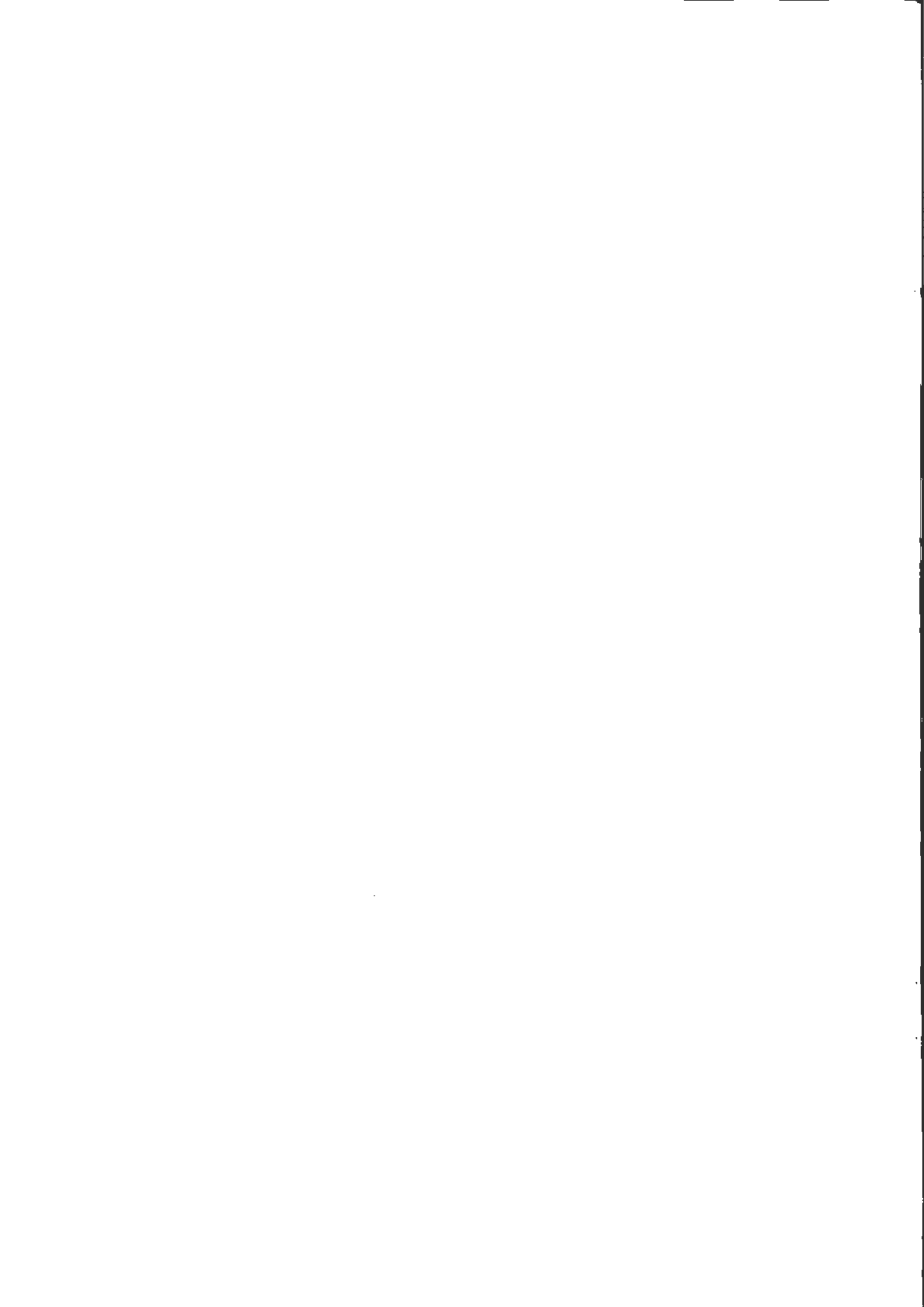


ANALYSIS OF CLIMATE-INDUCED HYDROCHEMICAL VARIATIONS IN TILL AQUIFERS

Sten Bergström, Per Sandén and Marie Gardelin



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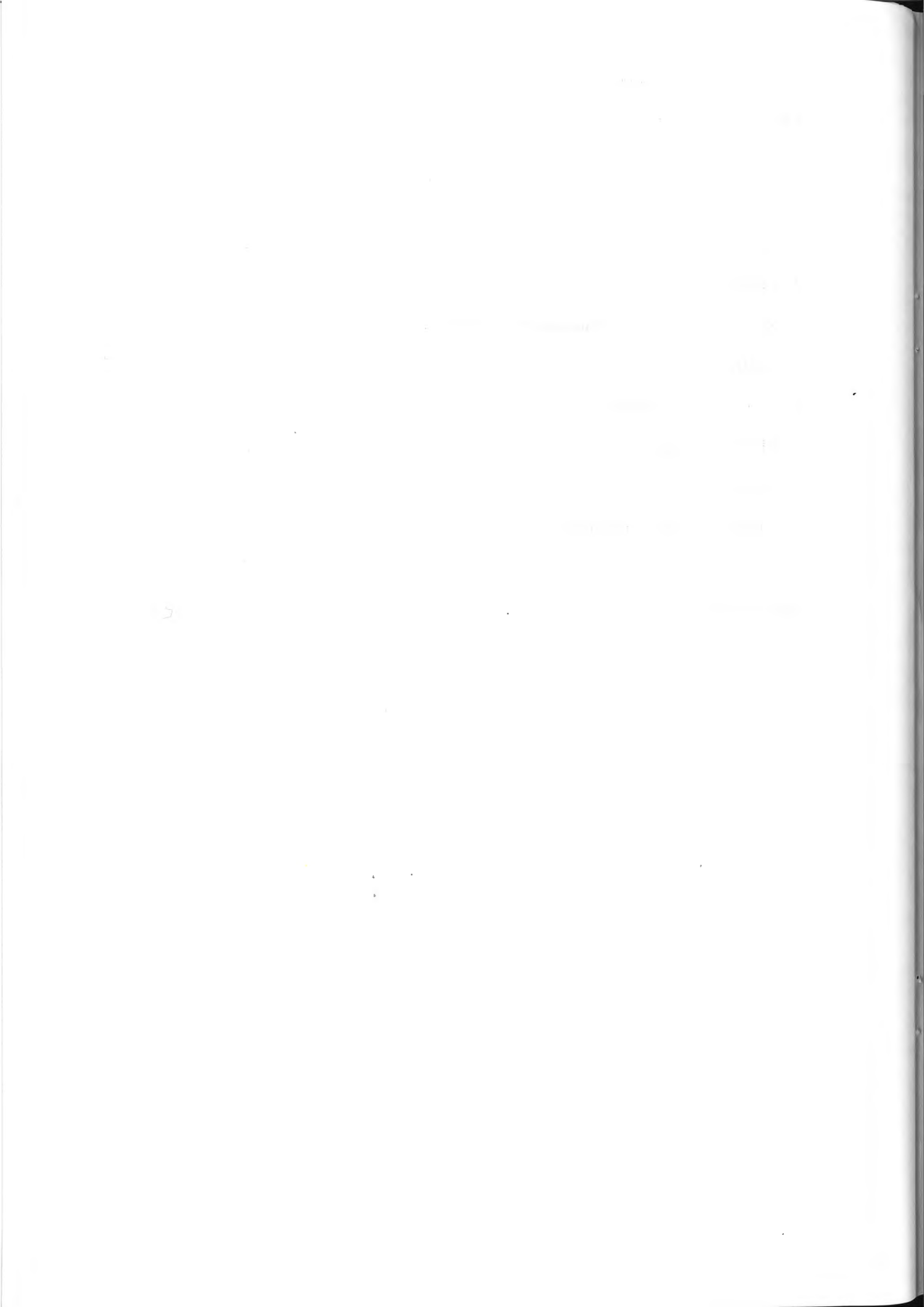
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ABSTRACT

An investigation of the relations between climatological factors and short term variability in groundwater storage and hydrochemistry in till aquifers is performed. The analysis is based on a simple empirical hydrological model, the PULSE model, and groundwater records from four sites in Sweden.

The model proved to be capable of describing the dynamics of groundwater levels or discharge, and at one of the sites it was possible to describe hydrochemical variations as well. The application to the remaining three sites illustrated that groundwater chemistry shows a much more complex pattern of variations than does corresponding streamflow in this type of basin. The importance of areal variabilities within the recharge area is discussed and illustrated by a distribution of the model into two submodels when applying it to one of the basins.

1. INTRODUCTION

Records of surface water quality often show patterns of variation, which are strongly related to hydrological conditions. The explanation is that the flow paths of water and thus their geochemical environment and mixing vary between wet and dry conditions (see, for example, Monitor, 1989). This concept has been used in the development of integrated hydrological and hydrochemical models, such as the ILWAS model (Gherini *et al.*, 1985) and the PULSE model (Bergström *et al.*, 1985). These model studies have shown that a surprisingly large proportion of the short term variation of pH and alkalinity in forest streams can be explained without any consideration of the quality of the precipitation or snowmelt. This is a significant result which can be used to separate short term variability from long term trends.

The simulation of long term variations of streamflow chemistry is a more complex problem that requires more advanced modelling approaches. One of the best known today is the MAGIC model (Cosby *et al.*, 1985), in which attempts are made to balance the effects of acid precipitation, ion exchange, weathering and streamflow

acidification. Another example is the Norwegian Birkenes model (Christophersen *et al.*, 1982). Although models of long term acidification are used extensively, questions still remain concerning confidence in the results of this type of models (see, for example, Bergström and Lindström, 1989). These questions will not be answered until we have hydrochemical records of enough length for model validation.

So far, most modelling exercises have mainly been oriented towards problems of surface water acidification. Concern has, however, also been expressed about possible ground water acidification, and then the question of natural variations due to climate fluctuations arises again. The aim of this study is thus to explore the possibility to use a hydrological model with simple empirical hydrochemical subroutines to describe natural short term variations in records of groundwater quality in relative shallow till aquifers in Sweden. The foundation is the PULSE model system described by Bergström and Sandberg (1983) and Bergström *et al.* (1985), which is a development of the HBV conceptual runoff model (Bergström and Forsman, 1973).

2. SPECIAL PROBLEMS IN GROUNDWATER MODELLING

The analysis of records of groundwater chemistry is more complex than is analysis of surface waters. First of all we have to consider the sampling site itself and what it represents. If we study water that has been pumped out of a tube, the level of the intake and the extension of the aquifer are prime variables (Figure 1). If the tube is relatively deep and the size of the intake is small, the groundwater quality can not be expected to vary much from one day to another. This is due to the slow exchange of water in the soil and thereby the longer time available to reach equilibrium in different types of reactions (ion exchange, complexation, precipitation, weathering, etc.).

The water quality in a spring, on the other hand, is expected to show a much greater short term variation which resembles that of a surface water stream. This is due to the different pathways of the dominating fraction of the water during wet and dry conditions. During wet conditions the main part of the water has passed

superficially in the soil, while dry conditions is dominated by water passing deeper in the soil, where both the residence time and the geochemical characteristics strongly affects the groundwater quality. The soil must, however, be of some depth if this relationship is to be expected.

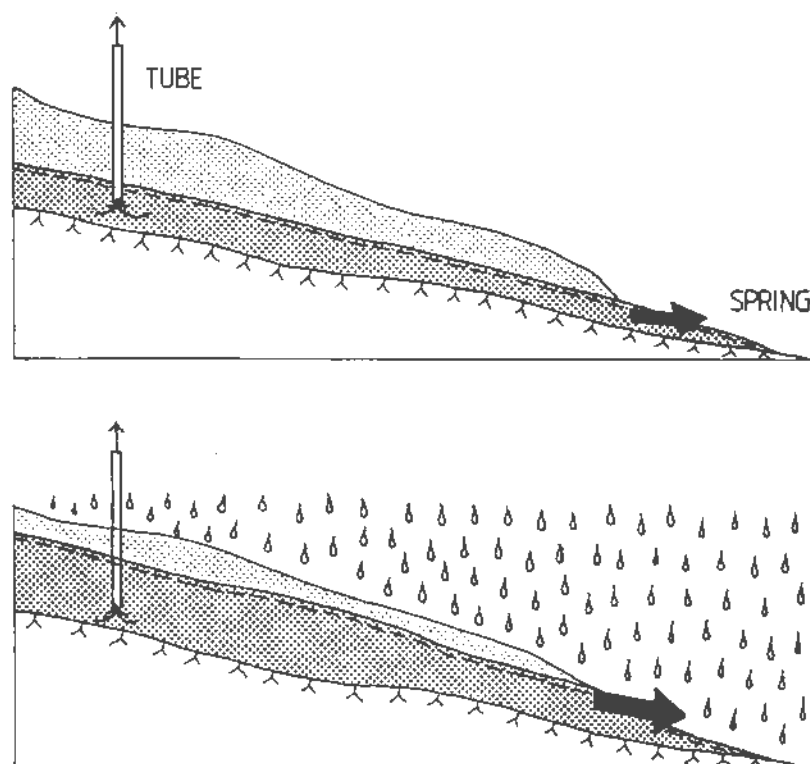


Figure 1. Principal sketch of the hydrological effects on groundwater quality. Superficial flow dominates the composition of the water in the spring under flood conditions, while the sampling point at the bottom of the tube is relatively unaffected.

When studying surface water quality we normally have a good idea of the extension of the river basin and can also measure streamflow continuously. This is not the case for groundwater chemistry. Therefore we have to master the water balance of the model indirectly by checking with records of groundwater levels or observations of flow out of the spring. This entails problems, as we have to make assumptions about specific yield at different levels of the aquifer and always will feel uncertain about the areal extent of the recharge area. Although it is relatively easy to calibrate the model to an acceptable agreement with observed groundwater levels or observed discharge, interactive errors between the water balance of the model and its hydrochemical components are thus more likely to occur.

3. MODEL STRUCTURE

The hydrological snow accumulation and melt routine of the water balance model is identical to that of the HBV model (essentially a degree-day approach), and so is the modelling of the unsaturated zone, with the only exception that capillary rise from the saturated to the unsaturated zone is considered.

The saturated zone is modelled according to the modifications introduced when applying the HBV model to groundwater observations (Bergström and Sandberg, 1983). This means that there is no limiting percolation capacity within the time step (24 hours), and quicker runoff can only occur when the groundwater level is high (Figure 2). This assumption is nowadays generally accepted for the relatively low intensities of rainfall and snowmelt in Sweden and the high permeabilities of till soils.

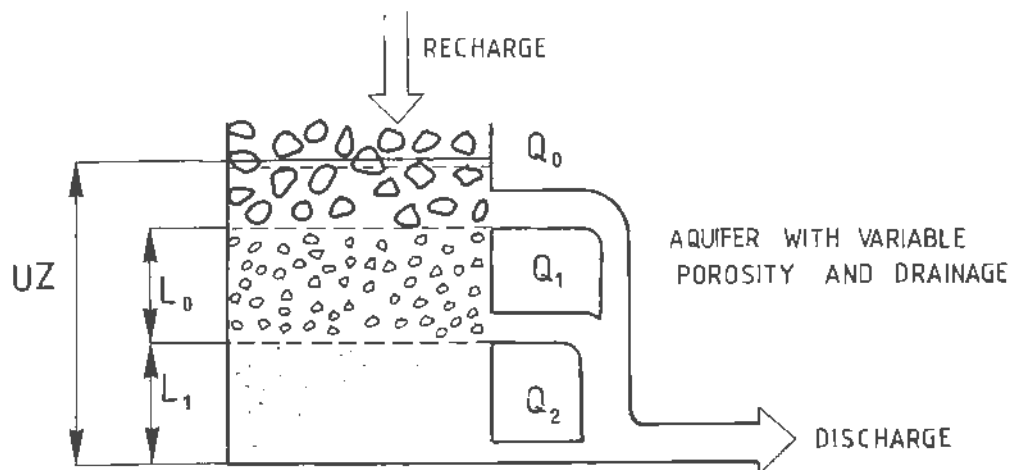


Figure 2. Outline of the drainage of an aquifer in the PULSE model.

To be able to compare recorded groundwater levels with simulations the model uses variable values of the specific yield with depth. This adds extra parameters to the model but is in agreement with general conditions of Swedish till soils (see, for example, Lundin, 1982). The specific yield is normally decreasing with depth.

A basic assumption in the model is that the quality of the discharge water is directly related to the level of the groundwater table in the modelled aquifer. The

justification for this assumption is the great chemical inhomogeneity which is persistent in a podzol profile. So is, for example, the surface of a forested till soil far more acid than deeper layers (Monitor, 1989). The general type of relationship between groundwater level and chemical composition is shown in Figure 3 and is in the model applied for all the chemical variables which we attempt to model. This subroutine entails the introduction of three model parameters for each one of the modelled elements (P_1 , P_2 , and P_3 in Figure 3).

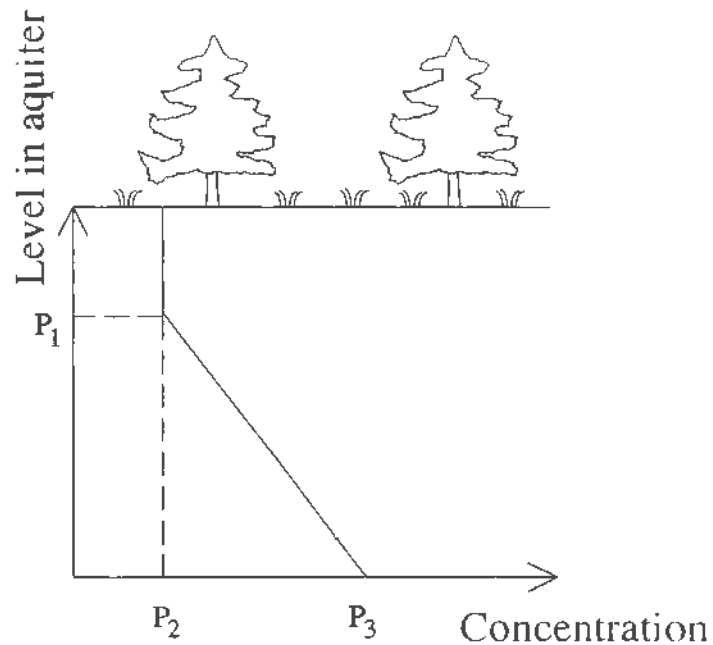


Figure 3.
Principal relationship between depth and water quality in the saturated zone of the PULSE model. P^1 , P^2 and P^3 represent parameters to be calibrated.

The final step in the simulations is the mixing of all contributions from the different levels of the discharged area and their corresponding concentrations. In general the superficial acid water will dominate during floods, in particular as this part has faster recession, while the chemistry of deep, less acidic, groundwater dominates low flow situations. The result is a pattern of variation characterized by rapid drops in pH and alkalinity during wet events and slower recovery during the recession period. Other modelled chemical elements will behave correspondingly.

It is important to note that the PULSE model is essentially a vertical one-dimensional model, which does not consider horizontal groundwater flow in any detail. It is further to be noted, once again, that the model only considers short term variations caused primarily by the dynamics of the groundwater table. No attempt is

made to model long term acidification of the system. This is the reason why the model only requires those input variables necessary for the water balance simulation, i.e. daily totals of precipitation, daily means of air temperatures, and monthly estimates of potential evapotranspiration. Chemistry of precipitation or snowmelt are not used as input to the model.

4. TEST SITES AND DATABASE

The model has so far been applied to two sites within the groundwater monitoring network of the Swedish Geological Survey (SGU), Dorotea and Nissafors (Figure 4). These two stations were selected after careful screening of several existing records. The hydrochemical records from Dorotea show an unusually strong seasonal variation pattern, which can easily be related to the regular winters and snowmelt seasons. The corresponding patterns from Nissafors are more difficult to relate directly to hydrological conditions, and this is more typical for other records from SGU, which were subject to screening. Both the selected sites have observations of groundwater levels in tubes and discharge water quality records from nearby springs. The groundwater level is recorded twice a month, while samples for analysis of water quality are normally collected four times per year.

During the snowmelt period of 1986 high frequency sampling has been performed by SGU in groundwater tubes at the Tiveden site (Figure 4). These data have been used in an attempt to trace effects on groundwater quality of a short intense melt period.

Finally, observations from a spring in the Stubbetorp research basin were used in the modelling exercise. These are from a temporary installation and cover only a short sampling period but have the advantage that records of discharge from the spring and a nearby precipitation station are available. The data from Stubbetorp are collected by SMHI and were of particular interest for studies of areal variability. The climatological database consists of daily totals of precipitation and daily averages of air temperature from the SMHI national network. Monthly averages of potential evapotranspiration were taken from Eriksson (1981).



Figure 4.
Geographical location of
the observation sites.

The predominant soil type at all sites is till, and the aquifers are relatively shallow and unconfined. They are all covered by coniferous forests.

5. MODEL CALIBRATION

Model calibration was performed in two steps. First the water balance part was calibrated by comparisons with groundwater levels in a tube that was considered representative for the aquifer. This means that parameters governing snowmelt, soil moisture dynamics and recharge were set together with recession coefficients and values of specific yield at different levels. For the Stubbetorp site the water balance was calibrated against discharge observations from the spring after having estimated its recharge area from maps and field surveys.

Once the water balance of the model was calibrated, optimal values were sought for the chemical model parameters for each element by comparison with hydrochemical records. That is, a relationship like the one in Figure 3 was specified by three parameters for each element separately.

The calibration process was based on visual inspections of the resulting plots, and no automatic optimization procedure was attempted. If the database was sufficient, split-sample technique was used, which is to say that a test period outside the calibration period was saved for independent verification of the model. The records from Stubbetorp were not considered of sufficient length for split-sample calibration.

6. RESULTS

A complete set of results for the test sites, Dorotea and Nissafors, are shown in Figures 5 and 6, respectively. As can be seen, the model describes the fluctuations of the groundwater level fairly well. As a matter of fact, some of the deviations are probably caused by poor observations of the groundwater levels rather than poor model performance. This is most obvious for Nissafors in 1982 (Figure 6).

The hydrochemical subroutine behaves relatively well for alkalinity, sulfate, calcium, and magnesium at the Dorotea site. Sodium and potassium show larger deviations, while the model is poor for chloride and nitrate. The results from Nissafors are much less encouraging for all elements. There are some noteworthy observations. Sulfate observations show a couple of extreme values. Nitrate seems to show a downward trend over the whole time period, 1971 - 1985.

Data from an intensive sampling period from four tubes at the Tiveden site were subject to a special analysis. As variability of these data proved to be low, we did not consider it worthwhile to try any detailed modelling. Instead we have chosen to visualize the modelled aquifer recharge together with observed hydrochemistry in Figure 7. In this case recharge is computed by the PULSE model with a standard parameter setting found reasonable from a large number of applications in the country. The four tubes represent two locations along a hill slope, and two different depth in the aquifer. As can be seen, there is very little response in the hydrochemical readings in spite of this relatively intense snowmelt event. The differences between the tubes are generally larger than the variation over the time period.

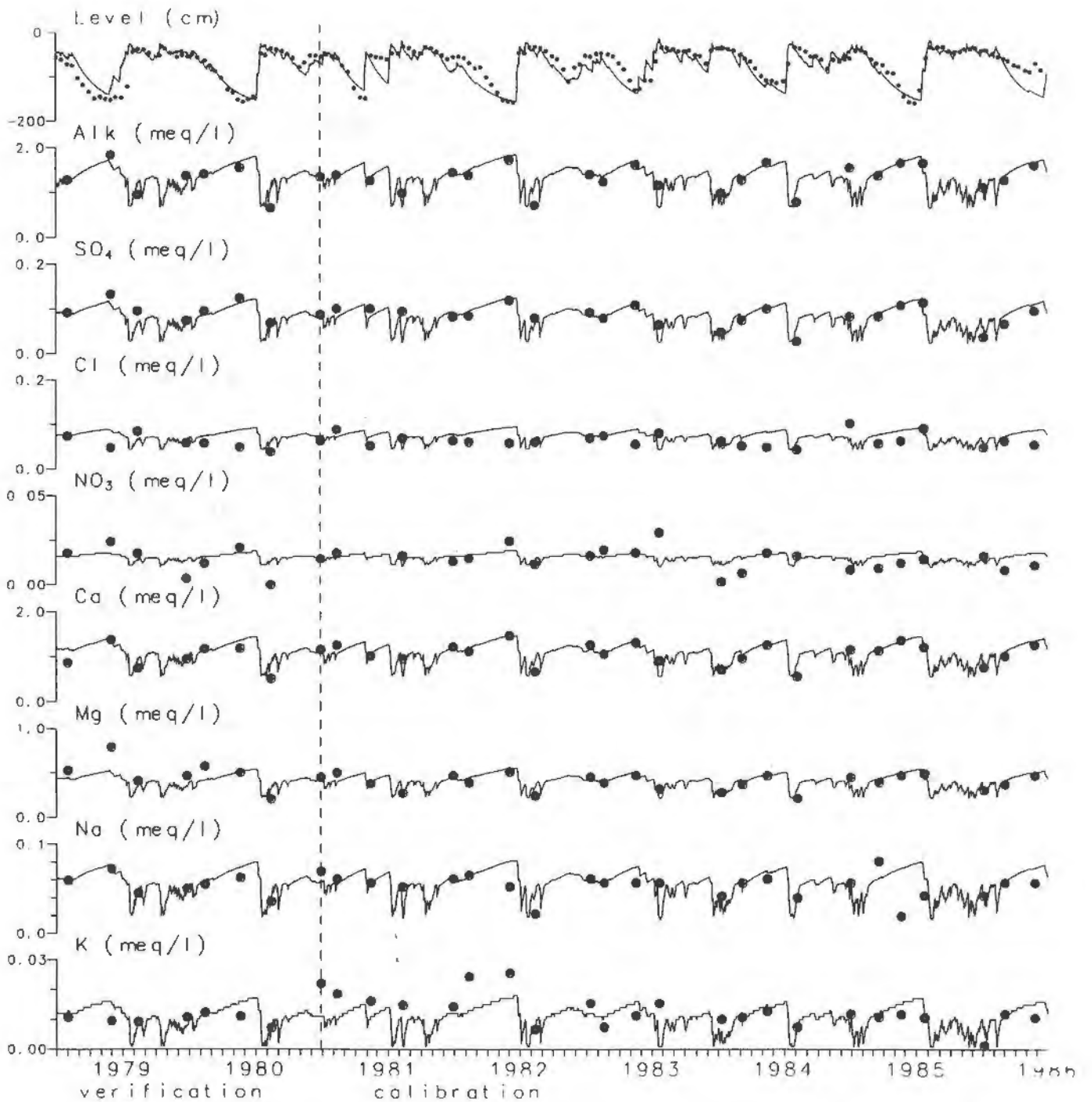


Figure 5. Simulation of groundwater levels and chemistry for a till aquifer at Dorotea. Dots represent observations and full lines simulations.

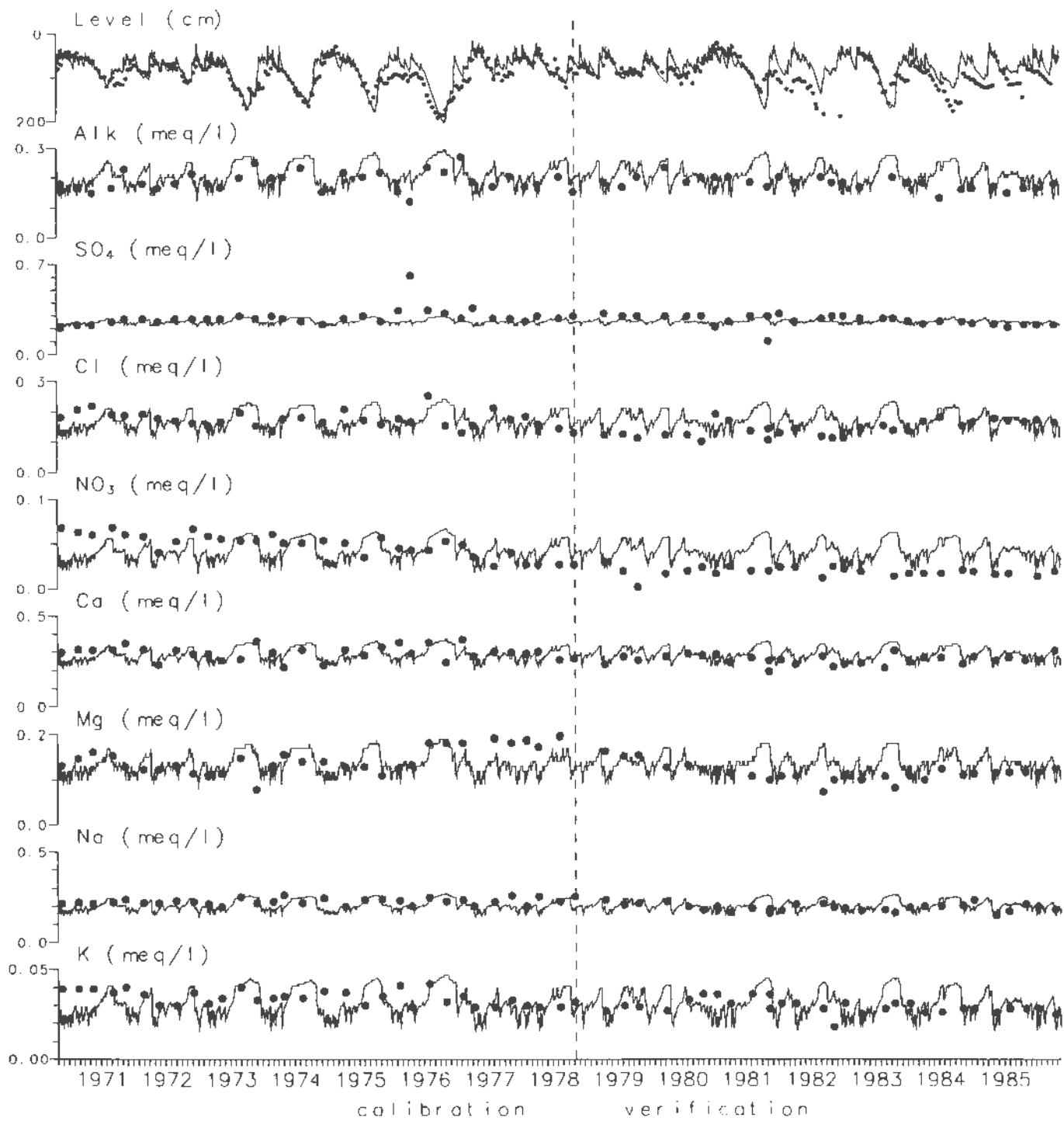


Figure 6. Simulation of groundwater levels and chemistry for a till aquifer at Nissafors. Dots are observations and full lines simulations.

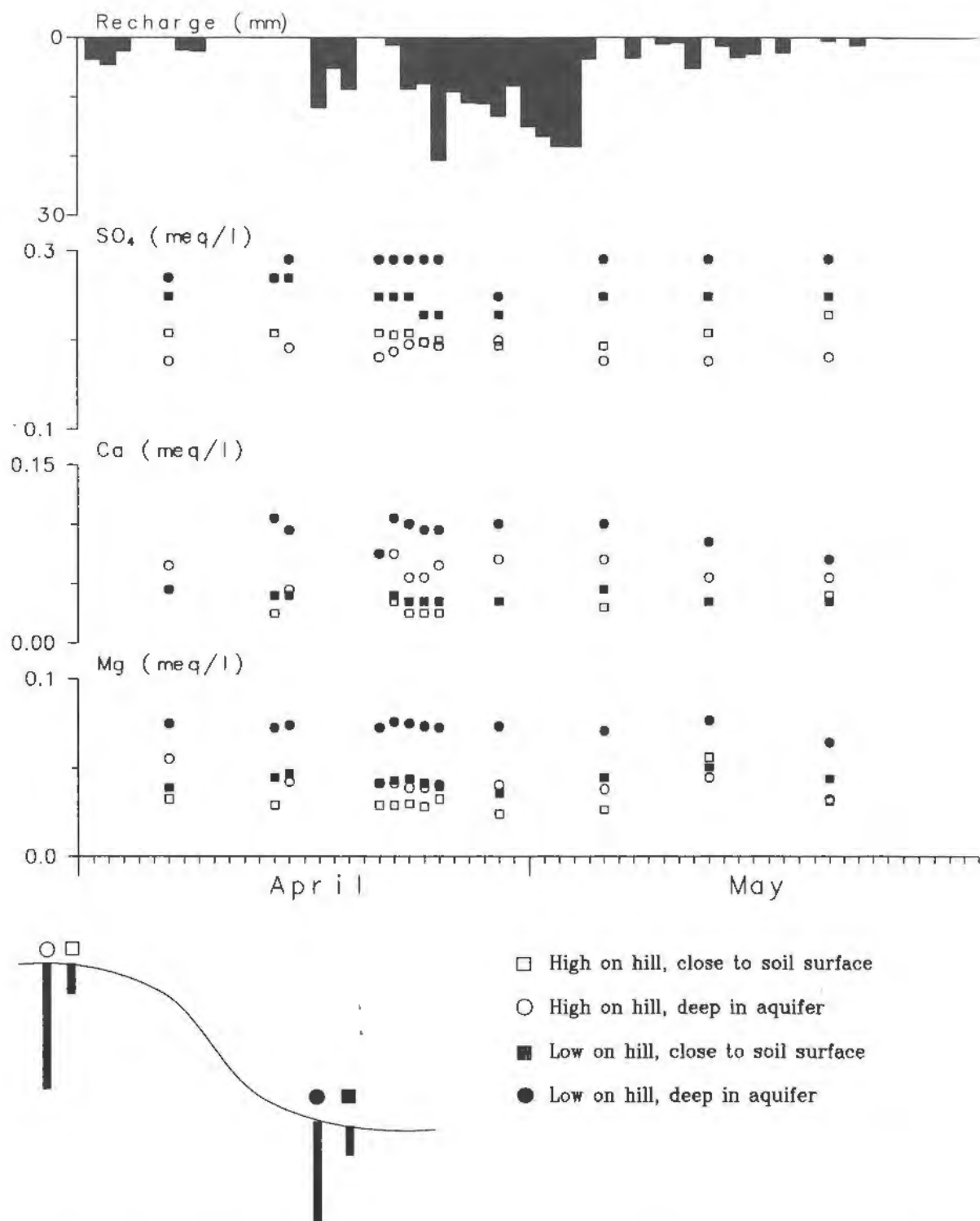


Figure 7. Simulated recharge and observed groundwater quality for four tubes at Tiveden during the spring of 1986.

The application of the model to the Stubbetorp site offered an opportunity to calibrate the model against discharge from the spring. It was felt that this application should show greater similarities to ordinary applications to smaller surface water streams. It was, however, soon realized that the simulation could not be successful unless a distributed approach was used. The original model consists of a relatively rigid link between discharge and alkalinity, which could only be found during winter and autumn conditions. During the dry periods in summer, acid surges were observed during flow events, in spite of a very low magnitude of these flood peaks. It was anticipated that these drops in alkalinity were caused by local areas with very thin soils and thus very low effects of soil moisture deficit in summer.

The model was therefore split into two submodels, one with an ordinary soil cover (80 % of the area) and the other with practically no soil moisture accounting capacity (20 %). This is in agreement with the actual conditions in the recharge area, which consists of roughly 15 % impediment and some areas with very thin soils. Even though this increase of complexity of the model can be justified by field surveys, it contributes to overparametrization of the model. In this case we are approaching, and maybe passing, a degree that can be accepted. Therefore the simulations (Figure 8) from Stubbetorp have to be regarded more as a theoretical study than as final results. Figure 8 shows a summary of the model simulation with the distributed model for the Stubbetorp site. As can be seen, the water from the larger area dominates the water quality during wet periods, while the practically soil-less area contributed mostly to acid peaks in summer.

Figure 8. Simulation of discharge and alkalinity from the spring in the Stubbetorp (opposite basin. Submodel A covers 80 % of the recharge area and has ordinary soil cover. Submodel B represents thin soils and impediment. Also shown separately for the two submodels are groundwater dynamics and alkalinity.

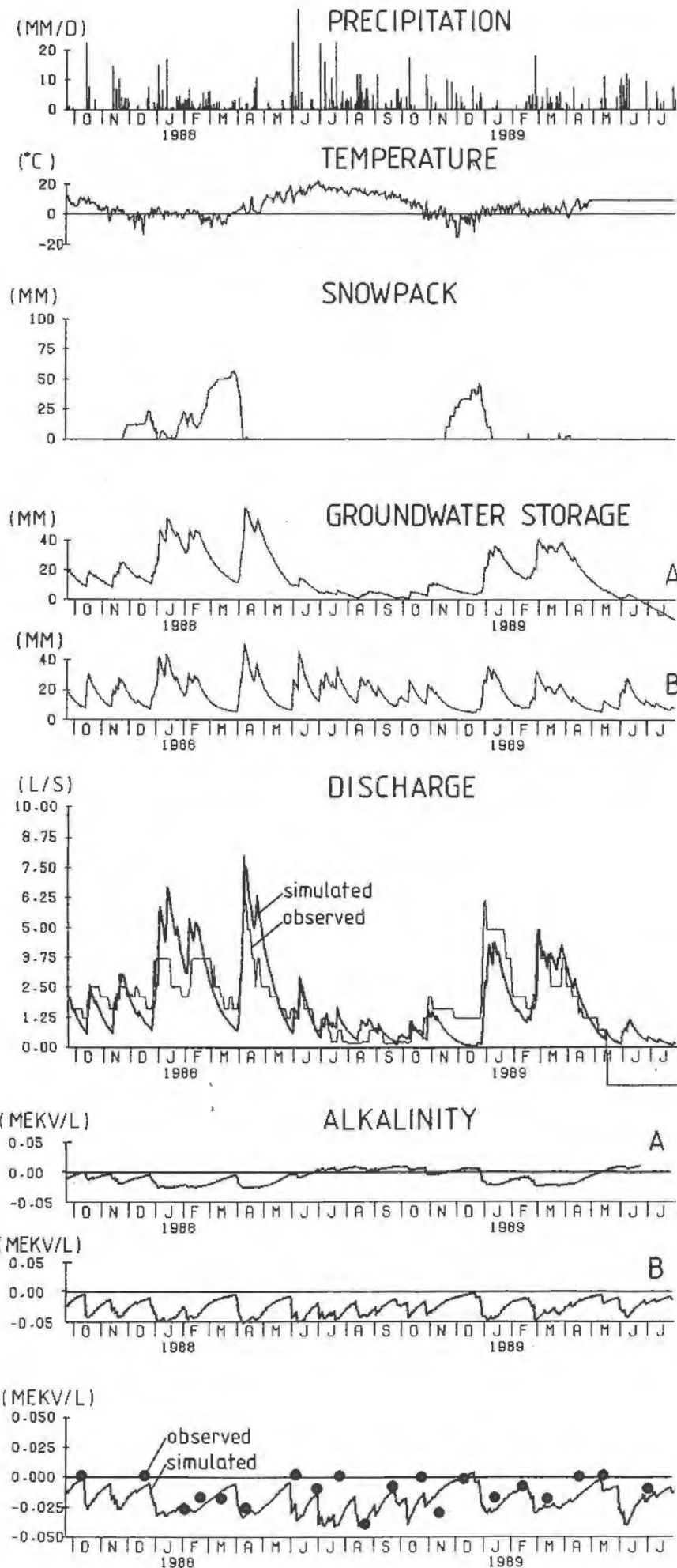


Figure 8.

7. DISCUSSION AND CONCLUSIONS

The conclusion that the PULSE model can be used for representation of groundwater response confirms what has earlier been shown in Sweden by Bergström and Sandberg (1983), by Johansson (1987) and in Finland by Lemmelä and Tattari (1988). The representation of levels has, however, to be interpreted with some care because of the many degrees of freedom. There is an obvious risk for overparametrization, when variable values of specific yield are allowed at various depth in the modelled aquifer. Nevertheless, there is little doubt that the main variability of recharge can be estimated by the model.

While it has been found that short term variations in forest stream hydrochemistry can often easily be attributed to flow paths and hydrological conditions, groundwater chemistry records are more intriguing. The results are contradictory for hydrochemistry of the two springs at Dorotea and Nissafors. While it was possible to simulate some of the elements in Dorotea, it failed for Nissafors. One explanation may be the difference in hydrologic regime. The Dorotea site is located within the mountain regime (Gottschalk *et al.*, 1979) with a more pronounced spring flood and less variability from year to year compared to the Baltic regime of the Nissafors site. It is clear that the main variation in chemical composition at Dorotea is due to a drop in concentration during the spring flood, while the rest of the year exhibits relatively constant values. Another explanation might be differences in the local hydrological conditions. Little variations can be expected if the water pathway to the spring is more or less the same during both wet and dry conditions.

It is further important to note the difference in average values and range between the two sites. This might indicate larger differences in soil physics and chemistry than was originally anticipated.

The screening of data from other groundwater stations within the national network indicates that the clear relationship between hydrological conditions and water quality at Dorotea is more an exception than a rule. Normally attempts to model

the chemistry will be equally difficult for most of the records as for Nissafors.

The low sampling frequency constitutes a major problem for this type of modeling. Much of the fast variations in concentration can not be verified. It would therefore be most valuable to obtain a time series with high sampling frequency, to study the relationship between hydrological conditions and hydrochemistry in groundwater.

The extreme values in the sulfate records at Nissafors are hard to interpret. They may be due to sampling or analytical errors, but the high values could also be explained by drought and thereby oxidation of normally reducing zones in the soil. The indication of a downward trend in nitrate concentrations is even harder to explain, when considering the increased concentrations of nitrate in deposition during the time period (Swedish Ministry of Agriculture, 1982). An increasing primary production could possibly be used as an explanation. Another possibility is, of course, inconsistent sampling or analytical procedures.

The readings in the four tubes at Tiveden support the general concept of the PULSE model. Water from deeper horizons in the aquifer have higher concentrations of calcium and magnesium than water close to the surface. This is true for both sites. In the same time, as we follow the hill downwards, the concentrations increase as well. The variation over time for the different horizons, represented by the intake to the tubes, is much less than the variation between the tubes. The almost undetectable impact of the recharge during the snowmelt on the water quality is a very clear illustration to the role of the unsaturated zone and pre-event water. This has been thoroughly investigated over the last two decades by natural environmental isotopes (see for example Sklash and Farvolden, 1979; Rodhe, 1987).

The application to the spring in the Stubbetorp area, finally, shows that some improvements can be made by a distributed approach. The introduction of subareas with different hydrological and hydrochemical properties rapidly introduces a risk for overparametrization of the model. In the light of the limited data available from Stubbetorp, the results must therefore be regarded as a theoretical study only.

The principle to match the water balance simulations with one type of observations (groundwater levels or discharge) and the modelled hydrochemistry with records of the water quality of discharge is a quite powerful one, as it reduces the degrees of freedom in model calibration. Still we feel that interaction between these parts of the model is a problem, in particular as model calibration against ground water levels entails assumptions about representativeness of the tube and specific yield at different levels in the aquifer. It is therefore strongly recommended that, in the future, a sampling scheme is introduced, where groundwater levels and chemistry as well as discharge, if possible, are measured simultaneously and that the areal representativeness of the level readings are checked carefully. It is further recommended that a higher sampling frequency is introduced, in particular during significant hydrological events, such as intense snowmelt and autumn floods.

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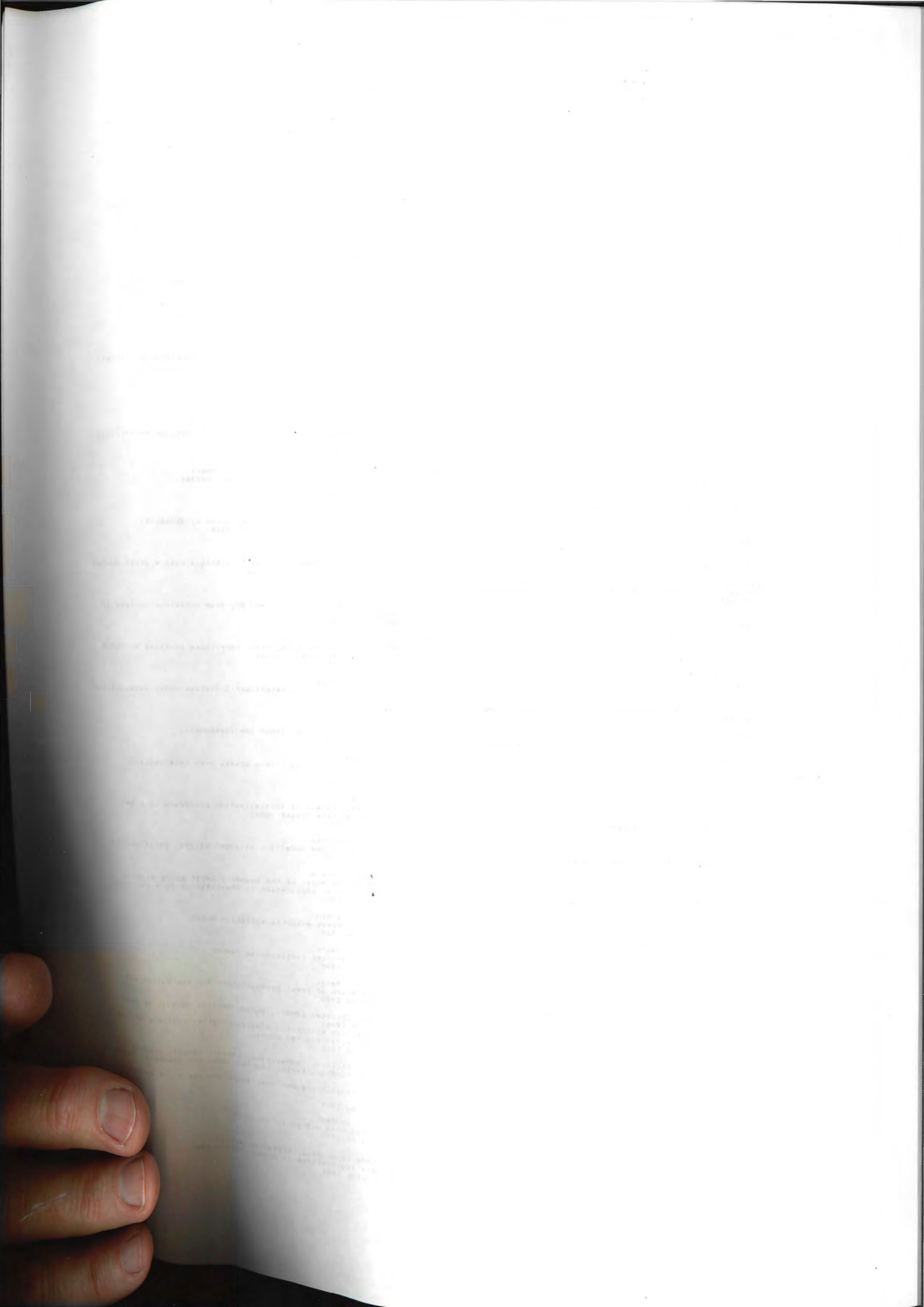
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