Nordic Hydrology, 22, 1991, 327-340

Spatial Variability of Physical Parameters and Processes in Two Field Soils

Part III: Solute Transport at Field Scale

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A numerical analysis of solute transport in two spatially heterogeneous fields is carried out assuming that the fields are composed of ensembles of one-dimensional non-interacting soil columns, each column representing a possible soil profile in statistical terms. The basis for the analysis is the flow simulation described in Part II (Jensen and Refsgaard, this issue), which serves as input to a transport model based on the convection-dispersion equation.

The simulations of the average and variation in solute concentration in planes perpendicular to the flow direction are compared to measurements obtained from tracer experiments carried out at the two fields. Due to the limited amount of measurement data, it is difficult to draw conclusive evidence of the simulations, but reliable simulations are obtained of the mean behaviour within the two fields.

The concept of equivalent soil properties is also tested for the transport problem in heterogeneous soils. Based on effective parameters for the retention and hydraulic conductivity functions it is possible to predict the mean transport in the two experimental fields.

Introduction

The movement and distribution of chemical solutes in the upper soil are important to both the productivity of the agricultural land and the quality of the environment. In agriculture an optimum application of fertilizers and pesticides is desirable from an economic point of view. On the other hand, the fate of these substances may pose a risk to ground and surface waters. Also seepages from landfills, industrial waste products, spills of toxic chemicals during transportation *etc.* constitute a threat to the groundwater quality. The unsaturated zone is a key element in relation to these problems, and to predict the risk and extent of groundwater contamination a thorough understanding of the processes in this zone is required.

The physical processes of transport and dispersion of soluble substances in the unsaturated zone are governed by the movement of the soil water, and, as discussed in Part I and II (Jensen and Refsgaard, this issue), water movement exhibits a large degree of spatial variability as a result of soil heterogeneity. Consequently, also solute concentration is expected to vary in space, which complicates the description of solute transport in field systems and hence the assessment of pollution risks and agricultural management.

The traditional approach to describing solute transport involves the application of the classical convection-dispersion equation (CDE). This equation has been subject to numerous verification studies in the laboratory by performing displacement experiments in soil columns, and the success of these verification studies has motivated an extrapolation of this approach from the laboratory scale to field scale without any modification other than an appropriate increase in the dispersivity coefficient. As demonstrated in Part I (Jensen and Refsgaard, this issue) the classical CDE can provide useful results for the vertical displacement process at the local scale (*i.e.* field soil columns of small surface area). However, for the entire field the validity of this approach is questionable. Among others Bresler and Dagan (1981, 1983) showed that, under certain conditions, the profiles of the field-averaged concentration may differ considerably from those obtained by the convection-dispersion equation applied to an equivalent field characterized by effective properties. On the other hand, Schulin *et al.* (1987) found that the classical equation predicts the field-averaged concentration distribution reasonably well, and hence conflicting conclusions are present on the general applicability of this equation at field scale.

The disturbing factor is the heterogeneity of the natural soil formations, and this problem has led several investigators to interpret the field-hydraulic properties as realizations of random functions and hence also describe the solute movement over the field as random, see *e.g.* Bresler and Dagan (1983), Bresler *et al.* (1983) and Mantoglou and Gelhar (1985). However, as pointed out by Sposito *et al.* (1986) the manner in which the probability concepts should enter the description of field scale solute transport cannot be decided yet, because the existing experimental data are too sparse, and the detailed mechanisms by which solutes move through field systems are not well understood.

A prerequisite to obtaining a better understanding of water movement and solute transport on field scale is more field experimentation, and this demand has been one of the motivations for the present study.

Analysis af Solute Transport at Field Scale

As described in more details by Sevel *et al.* (1988) and in Part I (Jensen and Refsgaard, this issue) radioactive tracers were applied for studying solute movement in the field. The actual concentration profiles were obtained by a gamma logging technique.

The CDE coupled to Richards' equation was applied to the individual soil profiles within the two fields where data were available on both soil hydraulic properties, water content, suction, and concentration. Observed and simulated solute concentrations were compared for selected profiles in Part I (Jensen and Refsgaard, this issue), and as stated there the classical equation provides reasonable results for the profiles shown as well as for the remaining ones from which concentration data were available.

The tracer experiments were only carried out around a subset of the sampling profiles at the two fields (12 in Jyndevad and 6 in Taastrup), and hence a detailed statistical analysis of the horizontal tracer distribution cannot be justified on the basis of the available data. However, by assuming that the CDE remains applicable to all profiles in the fields, the more widespread information on the soil hydraulic properties can be utilized to predict the local solute movement at these locations.

The numerical analysis of solute transport at the field scale will follow the same framework as in Part II (Jensen and Refsgaard, this issue) by assuming that the fields are composed of an ensemble of one-dimensional non-interacting soil columns, each columm representing a possible soil profile. By distributing the hydraulic properties amongst the ensemble of soil columns according to the statistical distribution found in the actual field, the flow and transport in each column can be described deterministically using the two models which have proved applicable at the local scale. A subsequent statistical analysis of the predicted solute profiles can then provide estimates of the averaged concentration and variation in planes perpendicular to the vertical direction of solute transport. Such simple variables will, rather than the pointwise distribution of the concentration, exhaust the required information in most practical applications.

Similar to the flow analysis it is also here assumed that the statistical variation of hydraulic soil properties within the fields, both vertically and horizontally, is represented by the data from the 24 sampling profiles at the fields.

Jyndevad Site

The model analysis of solute transport is carried out by applying the transport model to all sampling profiles (24 in total) where the soil properties were measured. The same upper boundary condition is specified at all profiles corresponding to the field application of the radioactive tracer: instantaneous application of 100 μCi of ^{60}Co-complex over an area of 0.785 m^2 on December 7, 1984. As emphasized previously both transport and dispersion are assumed to take place in vertical direction only. For the longitudinal dispersivity a value of 8 cm is adopted.

In Fig. 1 the model-simulated radiation levels (pCi/g soil) based on soil properties from 24 sampling profiles are compared to measurements from a subset of 12 profiles. In the figure the simulated range of variation is bracketed by the current minimum and maximum values, whereas all measurements are shown individually.

Since the simulations include soil properties from a larger number of profiles than represented by the measurements, one would expect that the measurements are framed by the simulated range. However, this is not the case. For all levels shown in Fig. 1 it seems that the measurements exhibit a larger horizontal variability than shown by the simulations. Although part of this discrepancy can be explained by uncertainties in the logged radiations, the comparison clearly indicates that the water flow modelling, which essentially is the major part of any solute transport modelling effort, is not complete. These findings fit into the picture drawn in Part I and Part II of this study (Jensen and Refsgaard, this issue), where it was concluded that the variability of the water flow regime is not fully represented due to: 1) hysteresis in the retention function, 2) flow through macropores, 3) variable plant parameters such as leaf area index and root extraction pattern and 4) poorly defined hydraulic conductivity function.

Although the modelling procedure does not provide a complete representation of the observed variation in tracer concentration, the simulations capture the general trends of the solute displacement fairly well. At 10 cm depth the passage of the tracer pulse shortly after injection is simulated very accurately, and the model also seems to capture the recession characteristics in the following months. Also at 20 cm and 40 cm levels rather good simulations are provided of the overall displacement process. At the three following levels the deviations become somewhat more apparent; yet, the predictions reflect to a reasonable degree the overall observed displacement conditions, which justifies the application of the modelling procedure for the theoretical dispersion analysis described below.

Fig. 2 provides an alternative illustration of the simulation results which are still based on soil properties from 24 sampling profiles at the research field. The concentration is now expressed as radiation activity in the water phase, and the simulations have been extended deeper in the profiles to emphasize the dispersion characteristics. We have assumed that the soil characteristics measured at the lowest levels also apply deeper in the profile. The cross-hatched area also here represents the range of variation confined by the two extreme simulations, and as indicated by the figure the simulated horizontal variation tends to increase with depth. The continuous line represents the average concentration of all simulations over the field.

In the figure is further shown the simulation (as a dashed line) which is obtained by using effective soil parameters. These are established by averaging the retention properties arithmetically and the saturated hydraulic conductivity geometrically.

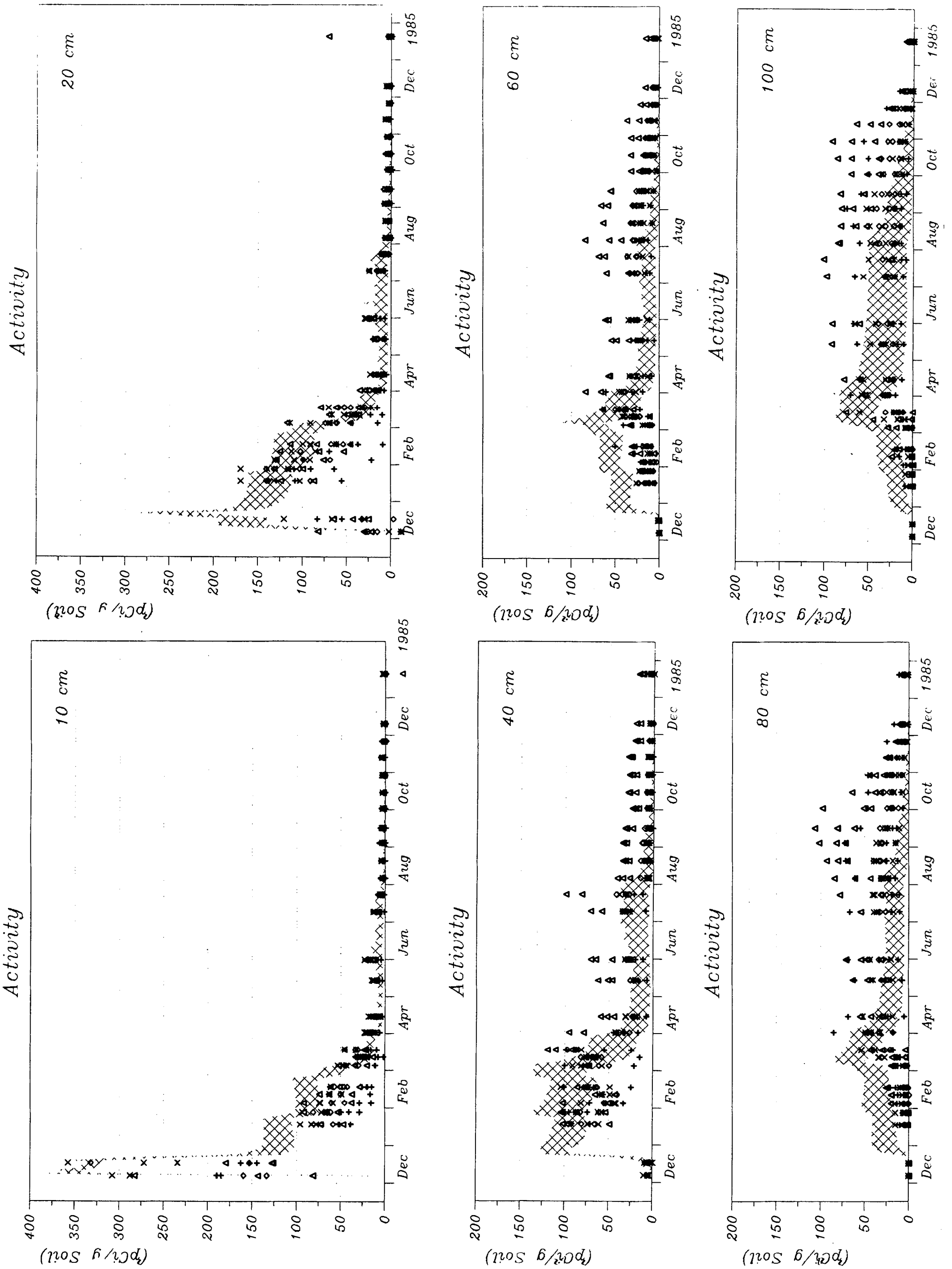

Fig. 1. Simulated range of variation in activity (cross-hatched) and individual measurements from 12 field points, Jyndevad site.

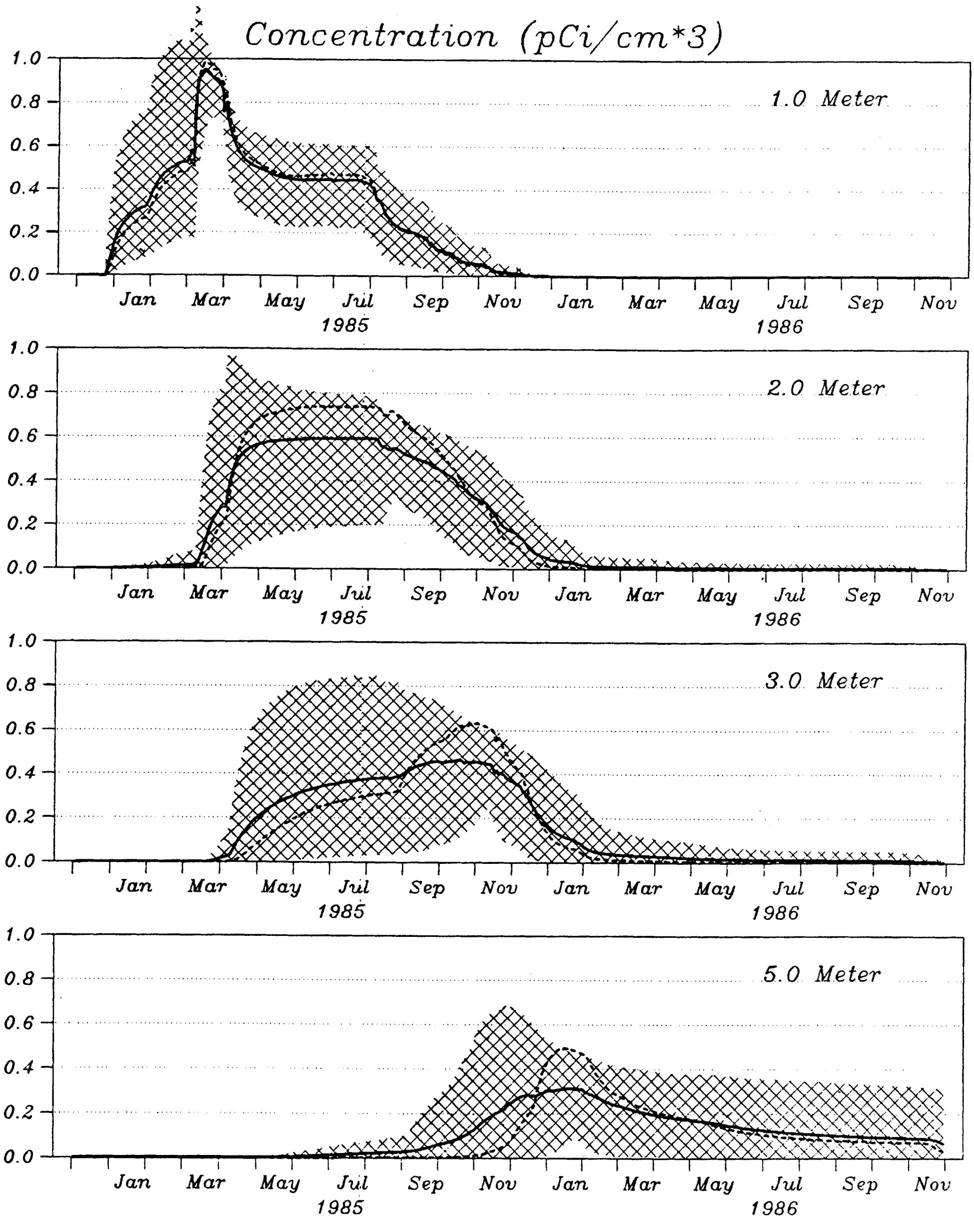

Fig. 2. Simulated range of variation in concentration (cross-hatched), average concentration (–) and simulated concentration based on equivalent soil properties (---), Jyndevad site.

For this particular simulation we used the same value for the dispersivity (8 cm) as for the individual columns. At the upper level (1 m) the equivalent model simulates the mean conditions very closely. However, at lower levels the simulation is not as

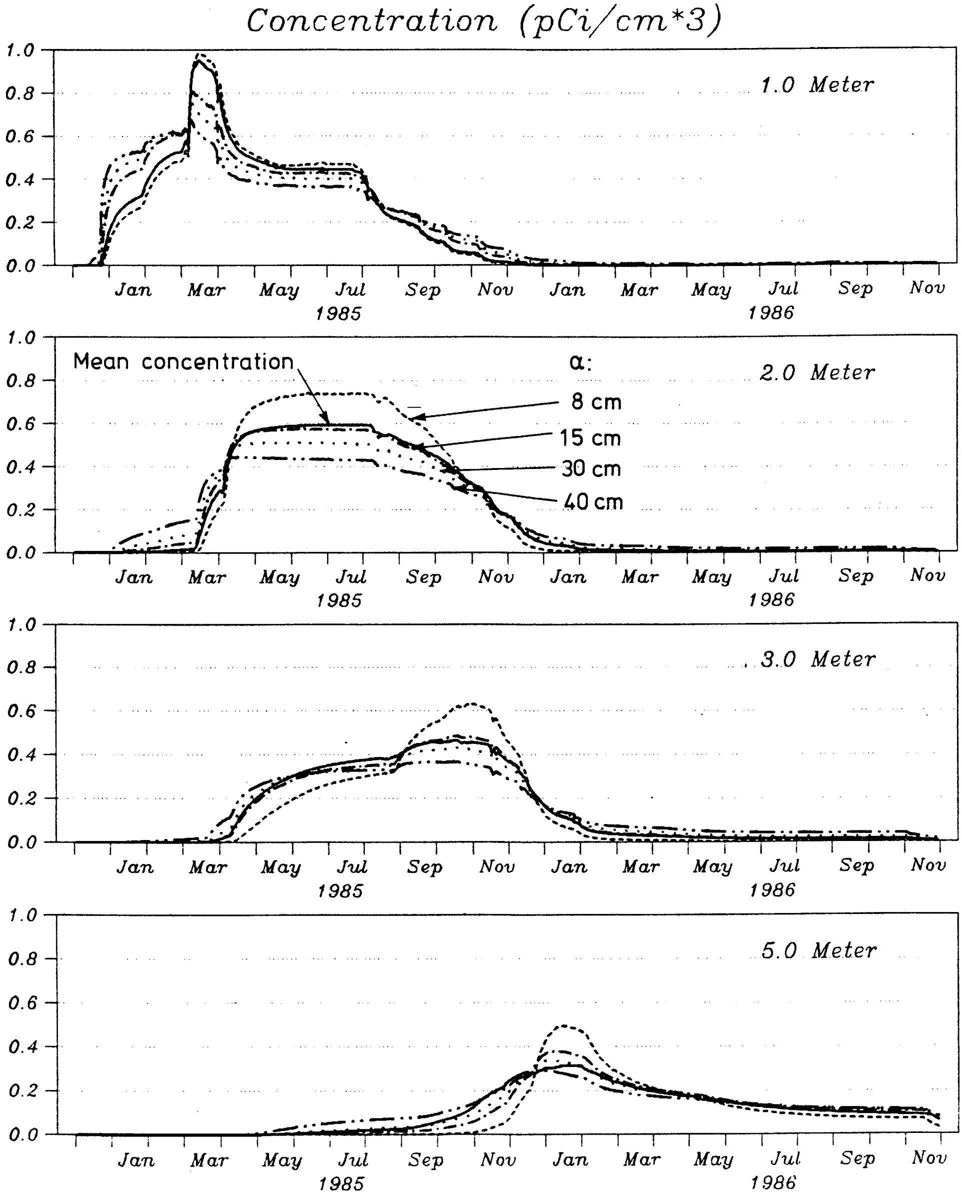

Fig. 3. Simulations based on an equivalent model with different values for the longitudinal dispersivity, Jyndevad site.

dispersed as the curves representing the mean concentration. This phenomenon is to be expected due to spatial variability in flow conditions over the field, which implies that the horizontal averaging over the field will result in a smoother breakthrough curve.

This effect can be compensated for in the equivalent model by increasing the dispersivity. Fig. 3 presents simulation results which are obtained by using the following values for the longitudinal dispersivity 8, 15, 30 and 40 cm. As shown by the figure the simulations approximate the field-averaged concentrations more closely deeper in the field when the dispersivity is increased. The results suggest that the larger the travel distance is, the more the dispersivity should be increased, a phenomenon which also has been reported by several investigators, *e.g.* Gelhar *et al.* (1985). Yet, it is somewhat surprising that the dispersivity should not be increased to a much higher value (another order of magnitude) in order to compensate for the field variability when enlarging the simulation scale from point to field.

In conclusion, it appears that, within the constraints of the present model approximations, an equivalent soil model based on averaged soil properties may provide results of practical relevance for solute transport and dispersion.

Taastrup Site

For this field site the same model analysis has been carried out as for Jyndevad involving application of the transport model to 24 sampling profiles. The input mode for all profiles is an instantaneous injection of 171 μCi of ^{60}Co-complex over an area of 1.767 m^2, and for the dispersivity a value of 5 cm is used.

Concentration measurements as radiation activity (pCi/g soil) were only carried out at six profiles (Cl-C6) and these are compared to the simulation results in Fig. 4. The simulation results are shown as the range of variation bracketed by the current minimum and maximum values, while the measurements are shown individually.

As for the Jyndevad site the measurements generally show a larger horizontal variability than the simulations. Possible explanations for this phenomenon are given in the discussion of the Jyndevad results above. For the Taastrup site we may add the following more specific comments. Considering the activities at 10, 20, and 40 cm depths during the period December-February it appears from the measured data that some of the tracer is retarded at 10 cm depth instead of being transported further down in the profile as suggested by simulations. This phenomenon may be caused by macropore effects whereby some of the tracer located in the upper soil layers is bypassed by the infiltrating water instead of being transported downwards.

It should be emphasized that a significant change in the overall picture occurs after the 103 mm rainfall event on July 23, 1987. Firstly, the range of variation among the six simulated profiles increases significantly. This is caused by different hydraulic responses of the six profiles to the extreme rainfall event. Secondly, contrary to the simulations the measured data indicate that the tracers after July do not move beyond 60 cm depth. This may be caused by the presence of a shallow

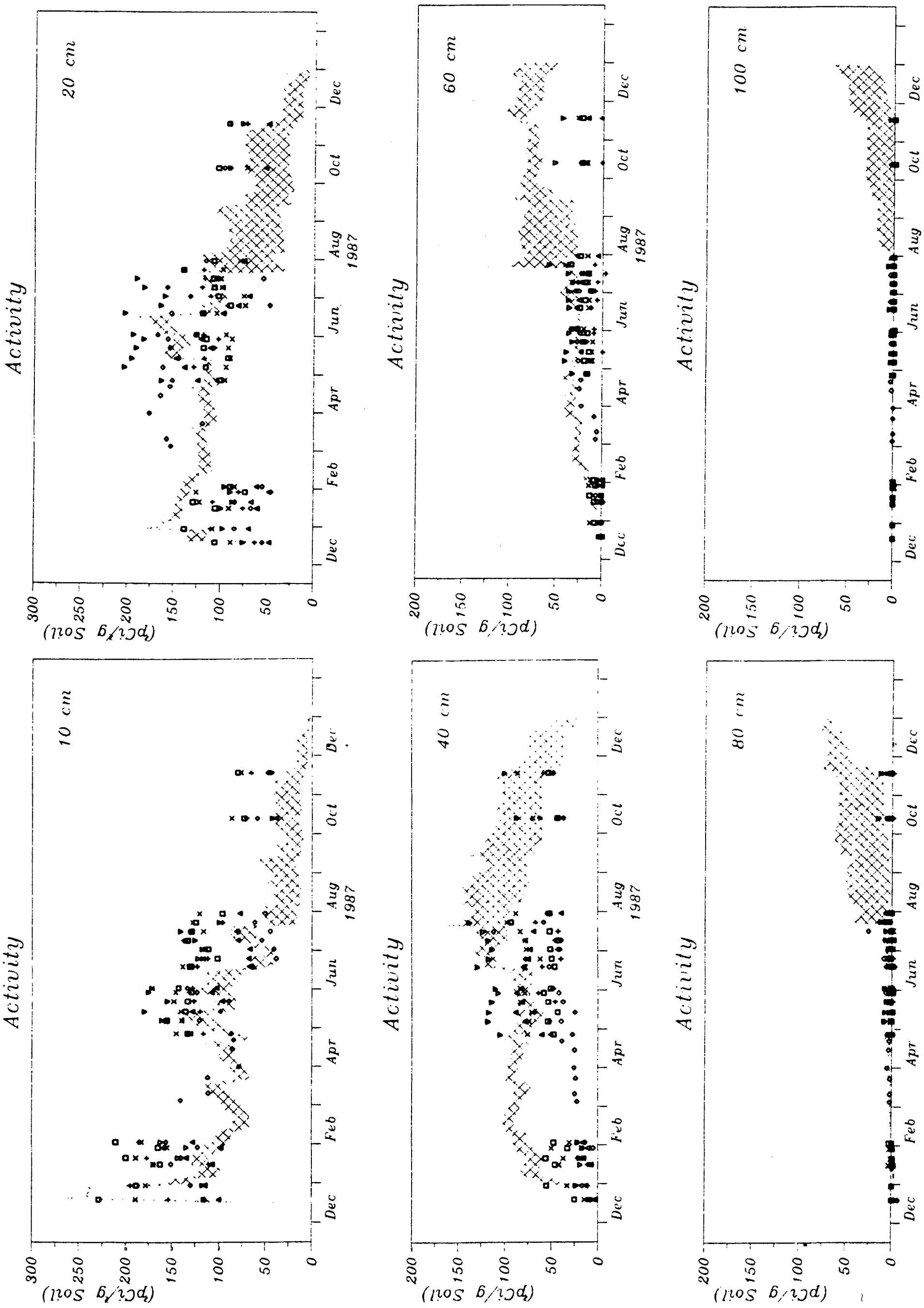

Fig. 4. Simulated range of variation in activity (cross-hatched) and individual measurements from 6 field points, Taastrup site.

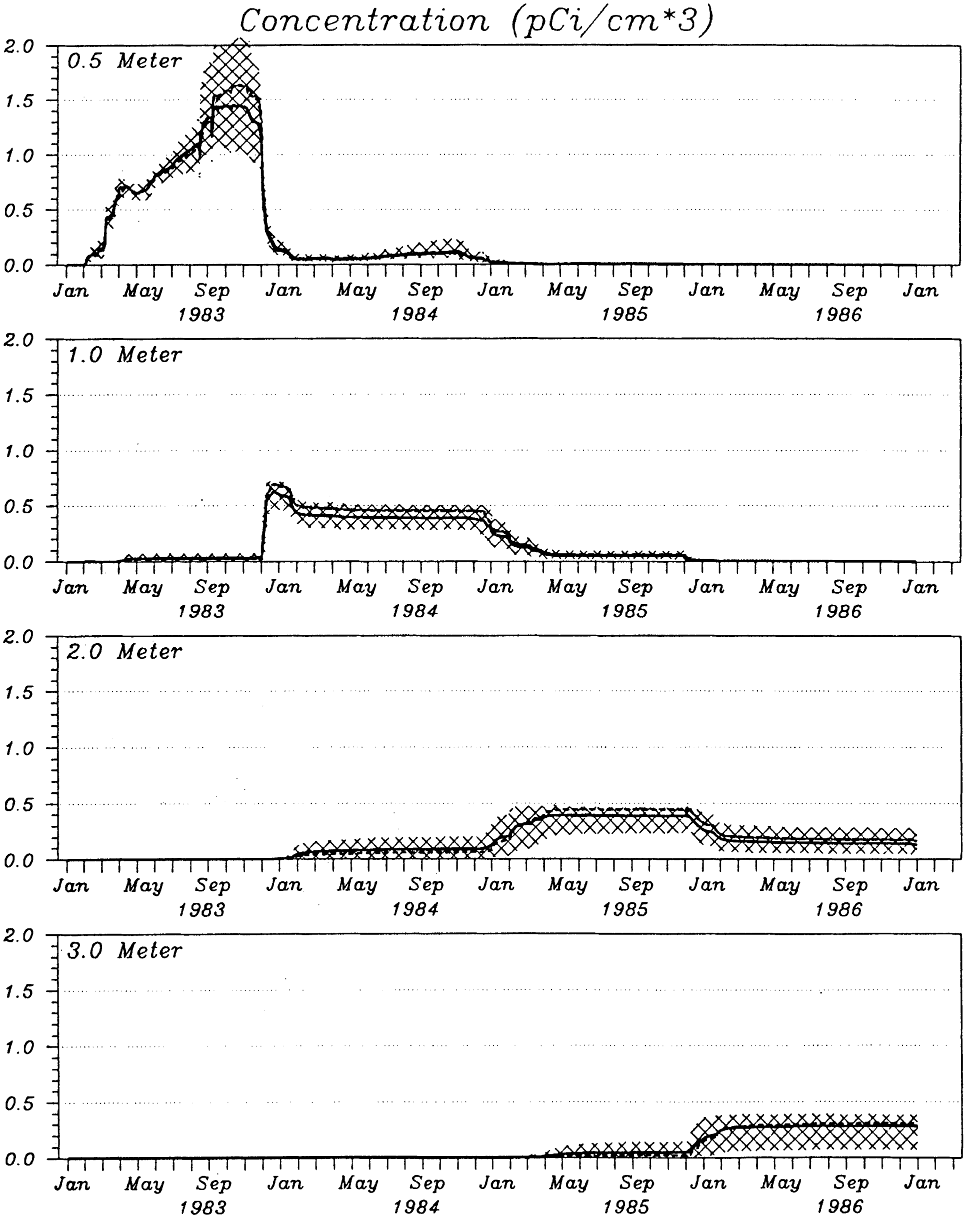

Fig. 5. Predicted range of variation in concentration (cross-hatched), average concentration (–) and predicted concentration based on equivalent soil properties (---), Taastrup site.

water table towards the end of July which may give rise to lateral transport of the tracer.

In spite of the discrepancies discussed above, the model simulations are able to describe the general trends of the solute displacement with a reasonable accuracy. At 10 cm depth the passage of the tracer pulse shortly after injection is simulated very well and also at 20 cm and 40 cm levels reasonable simulations are provided of the overall displacement process. However, at the three following levels the deviations become more apparent for reasons discussed above.

The number of tracer injection points were only six at Taastrup and due to an extremely wet summer in 1987 where the water table rose as high as to a level of 60-90 cm below the ground surface, the observed tracer movements can only be studied for a transport distance of about 60 cm. Therefore, in order to derive some general conclusions regarding dispersion at larger length scales, simulations were carried out for the 24 soil columns for a four-year simulation period, assuming the water table is located about 5 m below the ground surface.

Soil samples were not taken below 90 cm depth. In the following simulations, the soil properties measured at 90 cm depth for the specific field point have therefore been assumed valid onwards down to 5 m. Note that this assumption may tend to underestimate the spatial variation of the concentration profiles.

The simulation results are shown in Fig. 5 as break-through curves at four levels. The cross-hatched area represents the range of variation as reflected by the minimum and maximum among the 24 profiles while the mean is shown as a full line. Further, the simulation obtained by using effective soil parameters and the same value for the longitudinal dispersivity (5 cm) as for the individual soil profiles is shown as a dashed line.

In the upper layer a considerable variation of the concentration is noticed at the time of maximum concentration. In the lower layers this variation is not so pronounced in absolute values; however, relatively, the variation is increasing by depth indicating a gradual spreading (dispersion) of the injected mass.

The figure also shows that the simulation obtained by using effective soil parameter values does not deviate significantly from the mean of the 24 simulations. It seems that only a slight increase of the dispersivity parameter is required in order to describe the mean concentration for all levels, and it appears that the distance dependency is not present to the same degree as for the Jyndevad site.

Conclusions

The solute transport model which was calibrated on a few soil columns at two research fields was applied to simulate the transport of a conservative solute in 24 vertical soil columns at each of the two fields, where soil physical parameters were measured.

The simulated range of concentrations were compared to the observed values from 12 tracer injections at Jyndevad and 6 injections at Taastrup. For both sites the measurements generally showed a larger horizontal variability than predicted by the simulations. This was explained by 1) micro-scale spatial variations of soil properties in the field which are not accounted for in the soil parameter values applied in the model simulations, 2) noise in the observed data generated by the measuring and processing procedure, and 3) insufficient process descriptions.

For both field sites the model was extended to cover larger travel distances of the tracer, and the horizontal variation of tracer concentration was computed at various levels. The simulations showed that the horizontal variability tended to increase with depth in response to the ever increasing heterogeneity that the tracer plume will be exposed to.

A set of effective soil parameters was determined for both sites using a simple averaging procedure, and they provided a good description of the measured mean behaviour with only a slightly increased value for the effective dispersivity compared to the value for the local dispersivity. The simulations also showed that the effective dispersivity increases with the travel distance.

Acknowledgements

The present research project was carried out during the period 1984-1988 as a joint effort between five Danish institutes: Dept. of Soil and Water and Plant Nutrition at the Royal Veterinary and Agricultural University; Jyndevad Research Station from the Danish Research Service for Plant and Soil Science; Danish Isotope Centre; Danish Hydraulic Institute; and Institute of Hydrodynamics and Hydraulic Engineering at the Technical University of Denmark. The project has been financed jointly by the Danish Agricultural and Veterinary Research Council and the Danish Technical Research Council.

References

Bresler, E., and Dagan, G. (1981) Convective and pore scale dispersive solute transport in unsaturated and heterogeneous fields, *Water Resour. Res., Vol.* 17(6), pp. 1683-1693.

Bresler, E., and Dagan, G. (1983) Unsaturated flow in spatially variable fields, 3. Solute transport models and their application to two fields, *Water Resour. Res., Vol.* 19(2), pp. 429-435.

Bresler, E., Yaron, D., and Segev, A. (1983) Evaluation of irrigation water quality for a spatially variable field, *Water Resour. Res., Vol.* 19(6), pp. 1613-1621.

Gelhar, L. W., Mantoglou, A., Welty, C., and Rehfeldt, K. R. (1985) A review of field-scale physical solute transport processes in saturated and unsaturated porous media, Report RP-2485-05, Electric Power Research Institute.

Jensen, K. Høgh, and Refsgaard, J. C. (1991) Spatial variability of physical parameters and processes in two field soils, Part I: Water flow and solute transport at local scale, *Nordic Hydrology, Vol. 22,* pp. 275.

Jensen, K. Høgh, and Refsgaard, J. C., (1991) Spatial variability of physical parameters and processes in two field soils. Part II: Water flow at field scale, *Nordic Hydrology, Vol. 22,* pp. 303.

Mantoglou, A., and Gelhar, L. W., (1985) Large-scale models and effective parameters of transient unsaturated flow and contaminant transport using stochastic methods. Rep. 299, Ralph M. Parsons Lab., Mass. Inst. of Technology, Cambridge.

Schulin, R., van Genuchten, M. T., Flühler, H., and Ferlin, P. (1987) An experimental study of solute transport in a stony field soil, *Water Resour. Res., Vol.* 23(9), pp. 1785-1794.

Sevel, T., Butts, M. B., and Genders, S. (1988) Spatial variability of soil physical properties. Theoretical and experimental analyses. Radioisotope tracer studies, field measurements and analysis. Report Danish Isotope Center (internal report).

Sposito, G., Jury, W. Q., and Gupta V. K. (1986) Fundamental problems in the stochastic convection-dispersion model of solute transport in aquifer and field soils, *Water Resour. Res., Vol.,* 22(1), pp. 77-88.

First received: 26 March, 1991
Revised version received: 20 November, 1991
Accepted: 21 November, 1991

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