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Modelling of Unsaturated Flow in Heterogeneous Soils

Part I: Deterministic Simulations of Water Flow in Soil Profiles

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Water flow and solute transport in the upper soil layers are processes which are of importance in many hydrological and agricultural applications. These processes are occurring in a medium which has a complex composition, since the soil is a product of both the geological formation history and various man-induced activities like agricultural development. In addition, the upper soil is subject to cyclic variations in water content in response to the variable exposure of rainfall and outer evapotranspiration demand.

The paper describes simulations of the field conditions at different points within two research fields where comprehensive field investigations have been carried out. The simulations are based on solutions to the partial differential flow equation, subject to the measured climatic conditions and the hydraulic properties in the individual soil columns. The simulations of water content and capillary pressure are compared with measurements.

Introduction

The spatial and temporal variations of moisture conditions in the soil horizons above the water table play an important role in many areas within hydrology and agriculture, such as water balance calculations, irrigation and drainage, crop production, migration of pollutants etc. The moisture conditions in the unsaturated zone are determined by a number of interacting factors involving soil, crop as well as atmospheric processes which are difficult to separate and formulate in quantitative terms.

The level of the moisture content is to a large degree determined by the soil hydraulic properties, i.e. the retention and hydraulic conductivity functions, whereas the seasonal fluctuations are driven by the variation in rainfall and evaporative demand. Soil properties as well as climatic variables exhibit a spatial variation although the correlation scales are quite different. The correlation scale for climatic variables is much larger than for soil properties, and the present study focuses on the processes within a homogeneous climatological unit.

The study is part of a larger experimental and theoretical study which is carried out jointly by 5 Danish hydrological and agricultural institutes. The main objectives are:

- to investigate the magnitude of spatial variation in soil physical properties and variables within two fields belonging to two different mapping units representing a sandy and a loamy soil respectively.
- to evaluate the applicability of existing theories for predicting water flow and solute transport under field conditions.
- to develop appropriate methods for including variability and uncertainty in mathematical models.

Fig. 1 shows the field layout with the locations of the sampling and monitoring points (53 in total with variable distances between the individual points) within a rectangular area of 0.5 ha covered by grass.

A comprehensive laboratory and field measurement programme has been carried out including measurements of retention characteristics, saturated hydraulic conductivity, textural composition and continuous measurements of water content and tension. Some of these results have been summarized by Hansen *et al.* (1986). Further, radioactive isotopes have been injected at the soil surface around 12 sampling points for in-situ monitoring of the transport and dispersion characteristics.

The present paper discusses simulations of the moisture variations in the individual soil profiles on the basis of solutions to the flow equation subject to the appropriate boundary conditions and the parameters obtained from the soil analyses. The mathematical modelling analysis forms the basis for the following mathematical description of unsaturated flow characteristics over the entire heterogeneous field (Part II, Jensen and Butts 1986).

Model Components

Simulation of water flow in the unsaturated zone involves the flow components shown in Fig. 2.

Soil Water Flow

Assuming that water flow in the individual sampling profiles is strictly vertical the differential flow equation for unsaturated flow reads

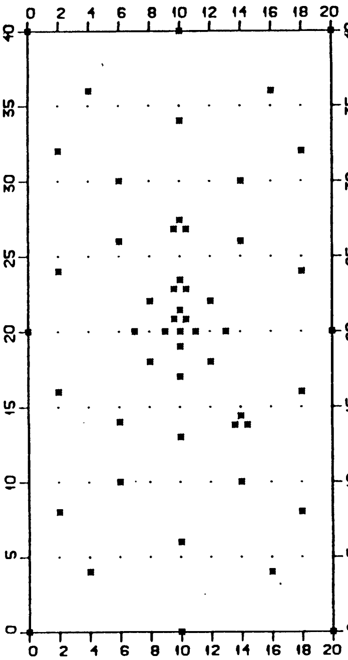


Fig. 1. Plan of field site showing locations of sampling points. (Coordinates unit: 2.5 m).

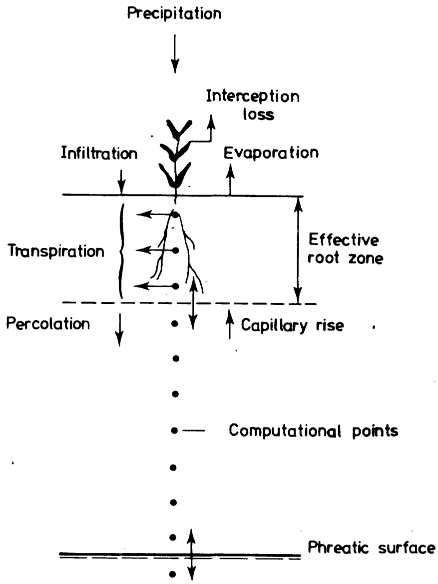


Fig. 2. Flow components in soil water flow dynamics.

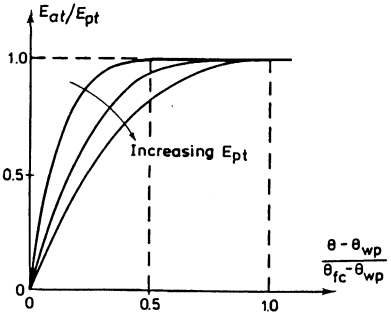
$$C\frac{\partial\psi}{\partial z} \equiv \frac{\partial}{\partial z}\left(K\frac{\partial\psi}{\partial z}\right) = \frac{\partial K}{\partial z} - S \qquad (1)$$

where

ψ – capillary pressure
C – water capacity
K – hydraulic conductivity
S – sink term representing uptake by roots
z – vertical coordinate, positive downwards
t – time

This equation is derived by combining the generalized Darcy law, in which the hydraulic conductivity is assumed to be a function of water content or capillary pressure, and the mass conservation equation.

Two functions are required for solving the equation: a) the retention function (relationship between moisture content θ and capillary pressure ψ) and b) the hydraulic conductivity function (relationship between hydraulic conductivity and moisture content θ or capillary pressure ψ). It is here assumed that these functions are not affected by hysteresis. For a further discussion of soil water flow dynamics, reference is made to Jensen (1983).



E_{at} – actual transpiration
E_{pt} – potential transpiration
θ – moisture content
θ_{fc} – moisture content at field capacity
θ_{wp} – moisture content at wilting point

Fig. 3. Relative transpiration as function of moisture content and potential transpiration.

Evapotranspiration

In any attempt to simulate naturally occurring moisture conditions in the field, the evapotranspiration processes will enter as essential factors. The evapotranspiration calculations are based on recorded values for daily potential evapotranspiration. These values are divided into a fraction absorbed by the vegetation and a fraction reaching the soil surface according to the following relationship, Jensen (1979)

$$E_{ps} = E_p \exp(-0.4\, L_{ai})$$
$$E_{pt} = E_p\, (1-\exp(-0.4\, L_{ai})) \qquad (2)$$

where

E_{ps} – fraction of E_p available for soil evaporation
E_{pt} – fraction of E_p available for evaporation of intercepted rainfall and transpiration
L_{ai} – leaf area index.

Part of the rainfall is intercepted on the vegetation surface from where it will evaporate directly. It is assumed that the interception capacity can be calculated from the relationship

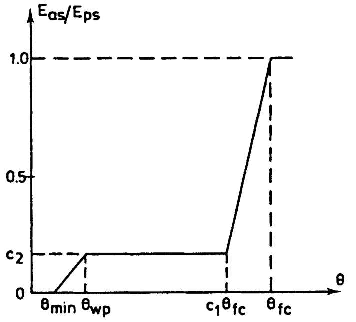
$$I_m = 0.05\, L_{ai} \qquad (3)$$

where

I_m – interception capacity (mm)
L_{ai} – leaf area index

The evaporative demand E_{pt} is first applied to the intercepted water and if it is not fulfilled the remaining part is applied for transpiration.

The external evaporative demand can only be met if the moisture supply in the root zone is adequate. For lower water contents the actual transpiration (root extraction) will be predicted according to the procedure illustrated in Fig. 3, Kristensen and Jensen (1975). This relationship is applied to all computational points



E_{as} – actual soil evaporation
E_{ps} – potential soil evaporation
θ – moisture content at the soil surface
θ_{fc} – moisture content at field capacity
θ_{wp} – moisture content at wilting point

Fig. 4. Relative soil evaporation as function of moisture content.

in the root zone and the derived values are subsequently multiplied by a distribution function to account for the extraction pattern of the root system. The values obtained hereby are introduced into the sink term S, Eq. (1). More details on the computational procedure can be found in Jensen (1983).

Similarly the soil evaporation demand is reduced below the potential value for moisture contents below field capacity, according to the procedure illustrated in Fig. 4.

The derived value for actual soil evaporation is also introduced in the soil water flow equation through the sink term S.

Boundary Conditions and Computational Procedure

The differential flow equation is solved by finite difference techniques on the basis of specified soil hydraulic functions and boundary conditions. Meteorological data are entered on a daily basis; however the time step in the numerical procedure is generally 1 hour or less in case of high rainfall intensity.

The model predicts for each time step the variation in the soil profile of water content, capillary pressure and water flow and velocity. Further, the actual values of interception loss, transpiration and soil evaporation are predicted.

Parameter Requirements

The modelling procedure described briefly above has been applied to several of the sampling profiles within the two fields with a view to establish a basis for modelling the flow in a heterogeneous field.

As a first approach it is assumed that vegetation characteristics described by leaf area index, root zone depth and root extraction pattern are spatially invariable. The same assumption applies to the observations of rainfall and potential evapotranspiration leaving the soil characteristics as the only parameters allowed to vary spatially.

Retention properties have been analysed in the laboratory on undisturbed soil cores removed at various depths (triplicate sampling). The moisture content –

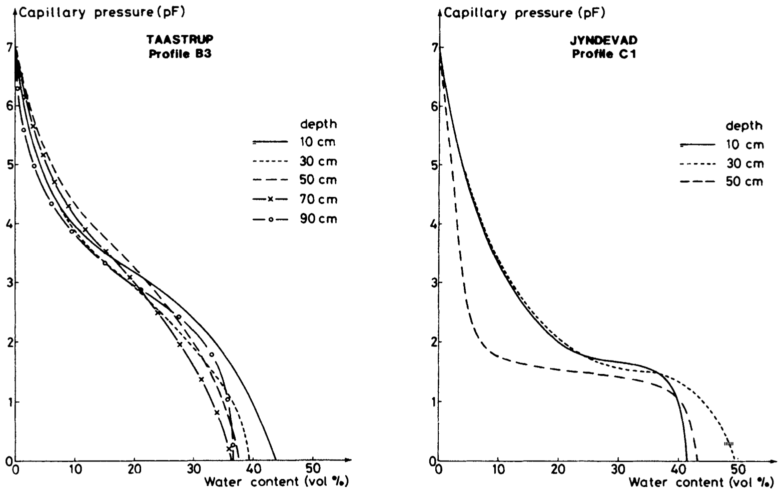


Fig. 5. Moisture content – capillary pressure relationships for a selected profile from each of the two field sites.

capillary pressure relationships representing a selected profile from each of the two fields are shown in Fig. 5. The difference in soil characteristies for the two fields are apparent from the curves: The Taastrup site has a wide pore size distribution and a high retention capacity whereas the Jyndevad site has a narrow pore size distribution and only little water is retained for tensions higher than 1.0 m.

Saturated hydraulic conductivity has been determined on undisturbed soil cores (triplicate sampling) taken from the same levels, whereas no experimental results are available so far on the hydraulic conductivity for lower moisture contents. The measurements have shown a very large degree of variability (see Hansen *et al.* 1986) even within the triplicates. The determination of saturated hydraulic conductivity on 100 cm^3 cores is apparently very sensitive to variations in pore geometry and in particular to incidentally occurring interconnected macropores. A variation of similar magnitude has not been observed for the other soil physical parameters.

In order to establish the complete hydraulic conductivity function, the concept of field capacity is utilized. Field capacity is the moisture content which is approached in the upper part of an initially wetted soil profile after a few days of draining by gravity forces. At this state no significant water flow occurs corresponding to a very low hydraulic conductivity. This value is here assumed to be approximately 0.3 mm per day. The moisture content at field capacity is generally found at a capillary pressure of – 1.0 m.

To describe the hydraulic conductivity over the whole moisture regime a power function of the following type is adopted, Mualem (1978)

$$K(\theta) = K_s \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^n \qquad (4)$$

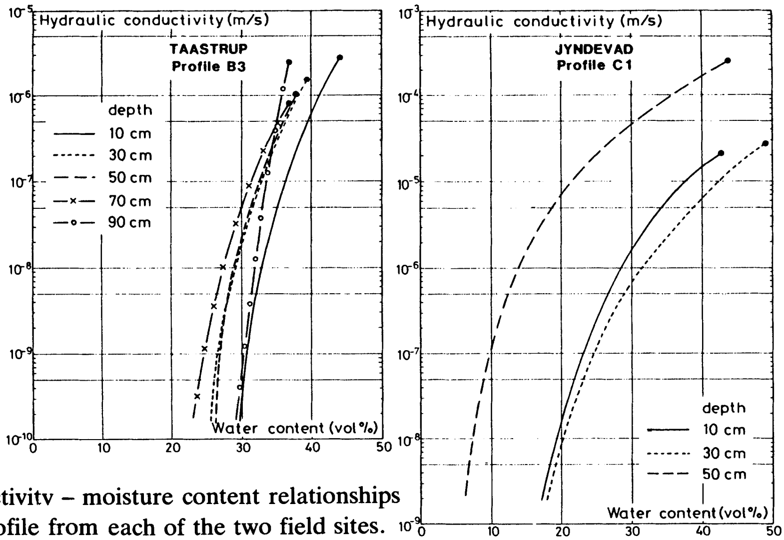


Fig. 6.
Hydraulic conductivitv – moisture content relationships for a selected profile from each of the two field sites.

where $K(\theta)$ – hydraulic conductivity at a given moisture content
K_S – hydraulic conductivity at saturation
θ – moisture content
θ_S – moisture content at saturation.
θ_r – residual moisture content.
n – exponent

The residual moisture content is the value where the hydraulic conductivity is effectively zero. It is here assumed that this value is obtained at pF = 3.0 (capillary pressure of – 10.0 m). The exponent n is subsequently calibrated on the basis of these assumptions.

In Fig. 6 is shown the adopted hydraulic conductivity functions corresponding to the profiles shown in Fig. 5.

Results and Discussion

Simulation results for the selected Taastrup profile are shown in Figs. 7-10 and for the selected Jyndevad profile in Figs. 11-14.

The simulation efforts presented here are based on the first data which have been processed from the research project. The field measurements of moisture content represent the only verification data available at present for the Taastrup site, whereas tensiometer recordings also have been processed for the Jyndevad site.

Generally viewed the simulation results are considered acceptable. For both sites the most obvious discrepancies in moisture content are present at the 10 cm level

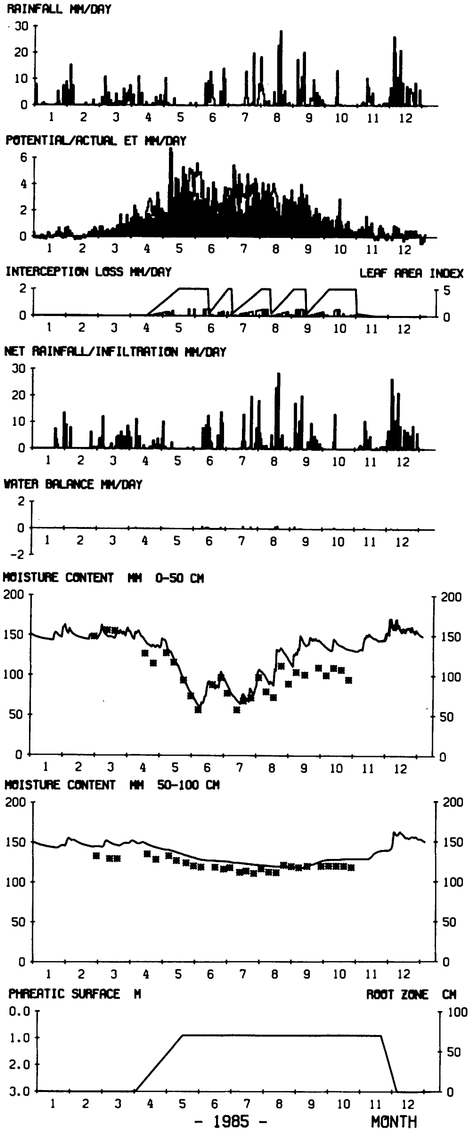
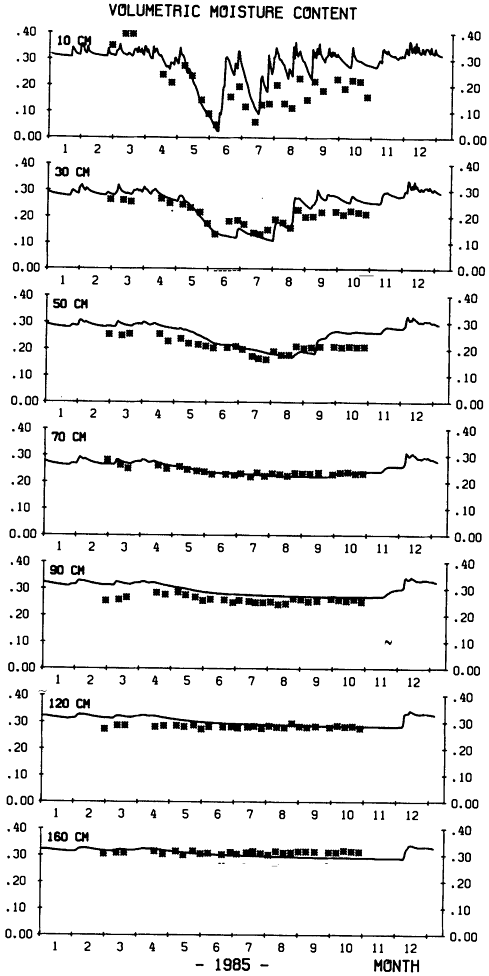


Fig. 7. Taastrup (profile B3). Input data, boundary conditions, evapotranspiration and soil moisture storage.



* Measured.
– Simulated.

Fig. 8. Taastrup (profile B3). Measured and simulated moisture content.

where the simulations overshoot the measurements in August, September and October. The discrepancies are likely to be attributed to deficiencies in the soil evaporation and root extraction procedure. However, the higher inaccuracy of the calibration curve for the neutron probe measurements close to the soil surface may also contribute to the discrepancies. This applies particularly to the Jyndevad site

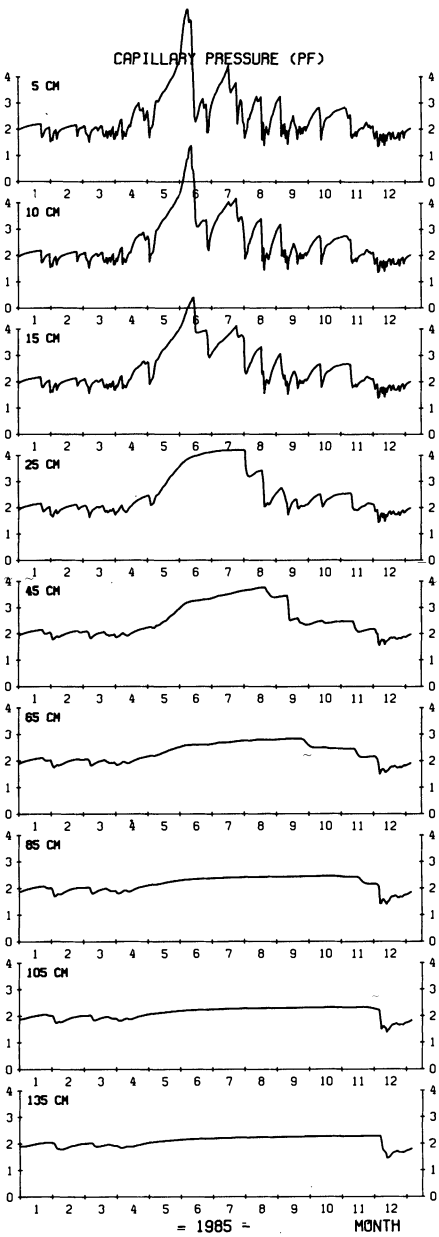


Fig. 9. Taastrup (profile B3). Simulated capillary pressure (logarithmic values).

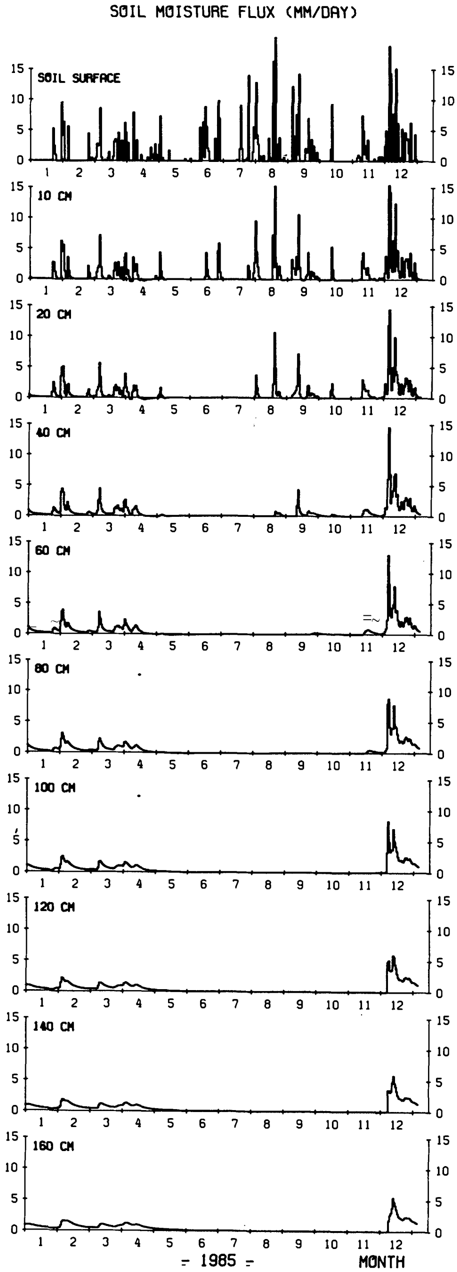


Fig. 10. Taastrup (profile B3). Simulated water flow (Darcy).

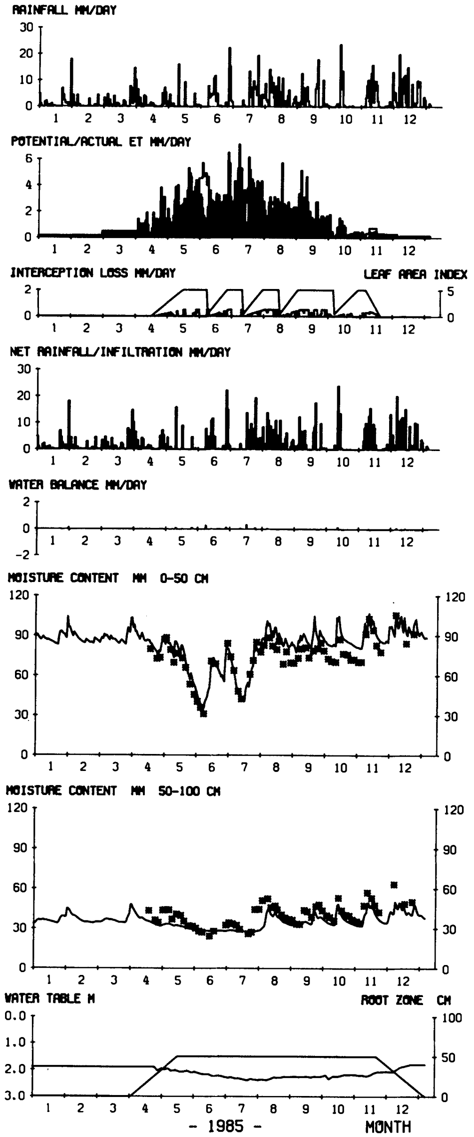


Fig. 11. Jyndevad (profile C1). Input data, boundary conditions, evapotranspiration and soil moisture storage.

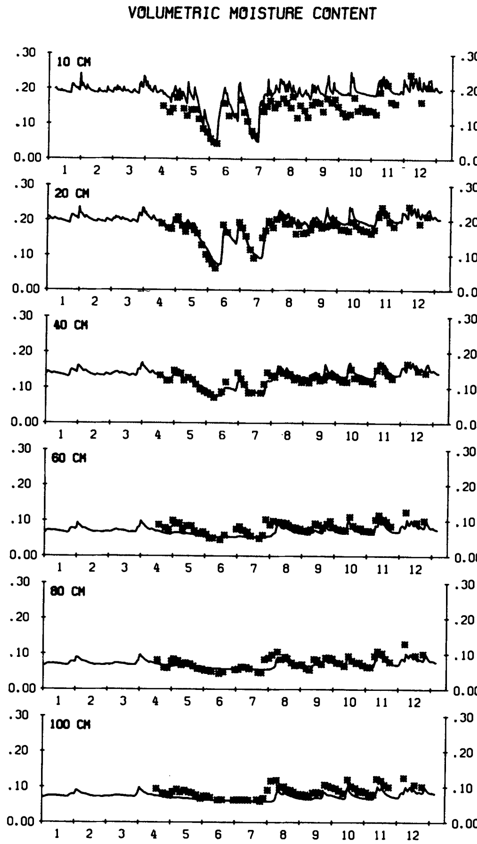


Fig. 12. Jyndevad (profile C1). Measured and simulated moisture content.

where the calibration curve has not yet been fully established.

Fig. 13 compares measured and simulated capillary pressures for the Jyndevad site. For the 20 and 40 cm levels a rather good agreement is obtained. Particularly the timing of the large changes in May, June and July can be emphasized. For the next three depths larger discrepancies are observed. These appear particularly in

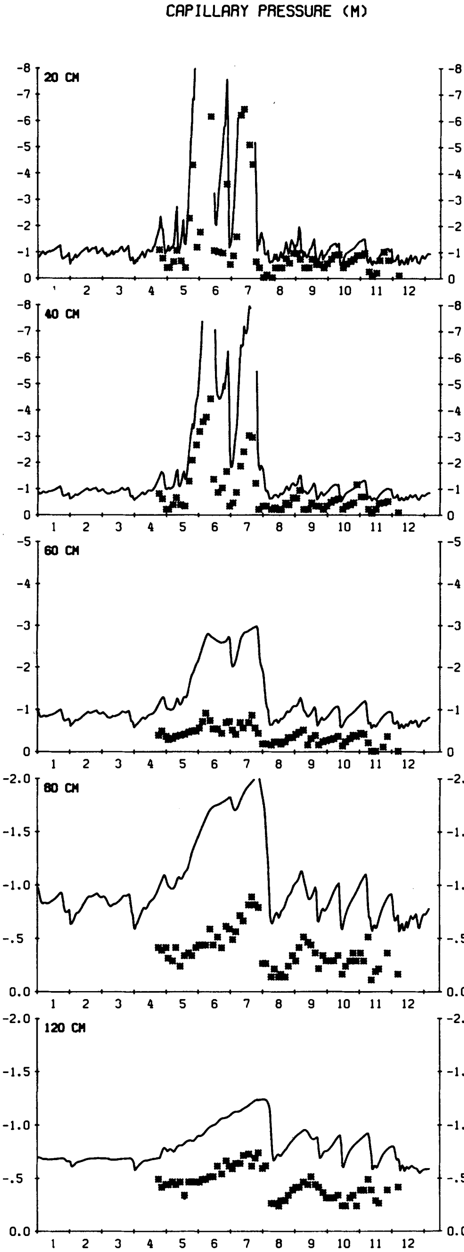


Fig. 13. Jyndevad (profile C1). Measured and simulated capillary pressure. * Measured. – Simulated.

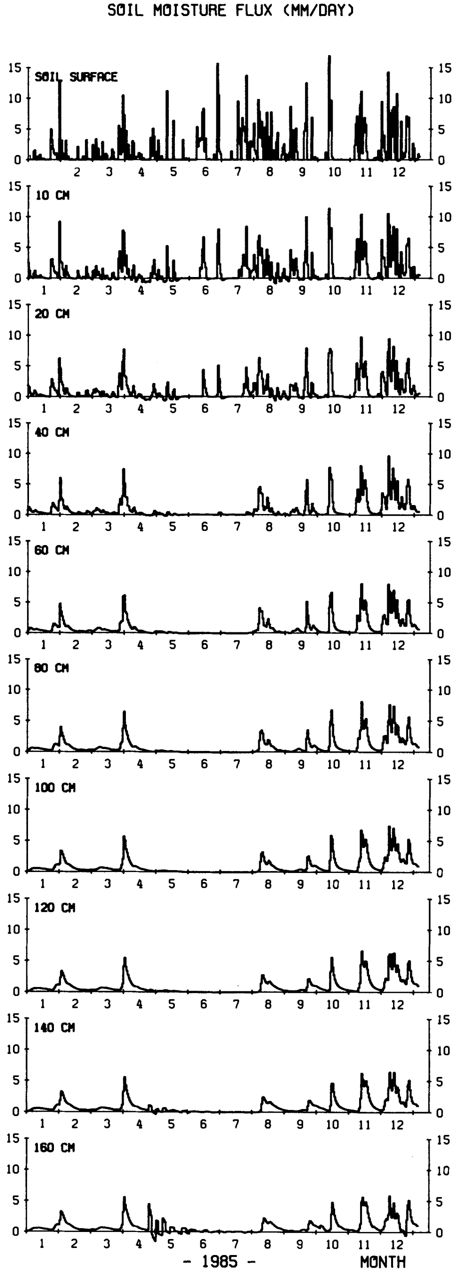


Fig. 14. Jyndevad (profile C1). Simulated water flow (Darcy).

the growing season where the simulated values are considerably higher. This should consequently imply that the simulated moisture contents are too low. However, this is generally not the case as seen from Fig. 12. This apparent inconsistency is partly due to the retention properties of this specific soil. For tensions higher than 1.0 m, large changes in pressure will only change the moisture content slightly and hence discrepancies will be much more conspicuous when shown on the pressure scale than when shown on the moisture content scale. Fig. 14 shows that the water flow (in upward direction) during the growing season between the 60 and 120 cm levels is almost negligible. However even this insignificant water flow is sufficient to give rise to the enhanced tensions shown in Fig. 13.

For the other sampling profiles within the two field sites simulations of similar quality has been obtained. As for the profiles shown here the discrepancies are predominant close to the soil surface and less pronounced in the lower horizons. As discussed above some of the discrepancies for the upper layer can probably be referred to the evapotranspiration modelling approach. In addition, the incomplete knowledge of the hydraulic conductivity function also contributes to the shortcomings of the simulations. For the lower horizons this is probably the main reason.

Despite these shortcomings, the described modelling approach will form the basis for the model analysis of the moisture conditions within the two heterogeneous field sites.

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