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CRACK - A MODEL OF WATER AND SOLUTE MOVEMENT IN CRACKING CLAY SOILS

Technical description and user notes

Nicholas Jarvis

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Rapport 159
Report

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PREFACE

This report describes a simulation model (CRACK) to predict water and solute transport in structured clay soils. The first section deals with the underlying philosophy and structure of the model and outlines the various interactions and feedbacks between component processes. It also gives a detailed description of how each component process within the model framework is treated in CRACK.

The second section deals with the input parameters required by the model, and puts considerable emphasis on evaluating alternative techniques for measuring, estimating or calibrating to obtain appropriate values.

The third section describes how to run the model on either IBM PC, XT, AT (or fully compatible personal computer), or on the VAX mini-computer. Several working examples of model runs (including input/output) are given in the appendices.

A few important model limitations are then briefly described, in the hope that model users may be dissuaded from unwise applications ! In the final section, possible future developments of the model are outlined.

If you would like to use the model, but have not yet obtained a copy on disc, please write to me at the address given on the back cover, specifying PC or VAX version. There will be a nominal charge to cover administrative costs. If you, as a model user, should find any bug that has so far been overlooked, I would be very grateful if you could report it to me (please write a brief summary of the problem and send it together with an exact copy of the input file that you used).

Finally, I would like to acknowledge Dr. Peter Leeds-Harrison (Silsoe College) for initiating and guiding the development and application of the model, and also Prof. Waldemar Johansson and Agr. Ingmar Messing (Department of Soil Sciences, Division of Agricultural Hydrotechnics and Soil Management) for helpful discussions and valuable comments on earlier versions of this manuscript.

Uppsala, December 1988.
Nick Jarvis

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INTRODUCTION

This report has been prepared as a guide for those wishing to use 'CRACK', a simulation model to predict water and solute transport in structured soils (primarily cracking clays). The driving force behind the development of CRACK was the realization that existing management orientated models could not satisfactorily account for the rapid 'by-passing' or macropore flow processes occurring in these soils. Such processes are known to influence, and may even dominate, the transport of water and dissolved substances (Thomas and Phillips, 1979).

A research project to develop such a model ('Water movement in swelling clay soils') was therefore initiated in 1984 at Silsoe College (a Faculty of Cranfield Institute of Technology) under a three year contract with AFRC (Agriculture and Food Research Council (U.K.)) and the supervision of Dr. P.B. Leeds-Harrison. Further development of the model has been carried out at the Swedish University of Agricultural Sciences, sponsored by NFR (Swedish Natural Sciences Research Council) since July 1988.

CRACK is a rather specialized model, but is also designed to be routinely applicable in the field on a seasonal/yearly time-scale. It is intended to be used as :

- a tool to improve our quantitative understanding of flow processes in the soil.
- an aid in interpreting results from field experiments.
- a guide to rational decision making in the field of soil and water management problems.

This report describes the model as of September 1988. As with any complex simulation model, it has undergone many transformations. If you are interested in tracing the development of CRACK and/or some early tests and applications of the model in the field, you are referred to Leeds-Harrison et al. (1986), Leeds-Harrison and Jarvis (1986), Jarvis and Leeds-Harrison (1987a,b) and Jarvis (1988a).

As the latest version of the model has only recently been developed, there are few examples, as yet, of validation of the full water balance model, or of the sub-model of solute transport.

In this report, you will find descriptions of :

- the conceptual framework of the model, and a technical summary of the main components.
- the input data required by the model, together with suggested techniques for parameter estimation.
- the mechanics of operation of the program on VAX or IBM (or fully compatible) personal computers, including some examples of input/output.
- limitations in the model and areas of possible future development.

TECHNICAL DESCRIPTION

CRACK models the water and solute balance based on a two-domain concept (i.e. cracks and aggregates) of transport in structured soils. The conceptual framework of the water balance model is best summarized by a flow chart (see Fig.1). A distinguishing feature of the model is the dynamic nature of the interaction between soil water content, soil structure and soil water flow. These feedback relationships between individual components of the model are explained in detail in the following sections.

Soil structure

A simple geometry is used to describe soil structure. The soil profile is divided into discrete layers (not necessarily of equal thickness), and each layer is assumed to contain cubic soil aggregates separated by planar cracks (see Fig.2).

The total porosity of the soil (e_t) is assumed constant and comprises two components, namely the crack porosity (e_c) and the matrix (i.e. aggregate) porosity (e_m) :

$$e_t = e_c + e_m \tag{1}$$

where

$$e_c = e_s + p(\Theta_f - \Theta) \tag{2}$$

and $$e_m = (\Theta + e_a) + \{(1 - p)(\Theta_f - \Theta)\} \tag{3}$$

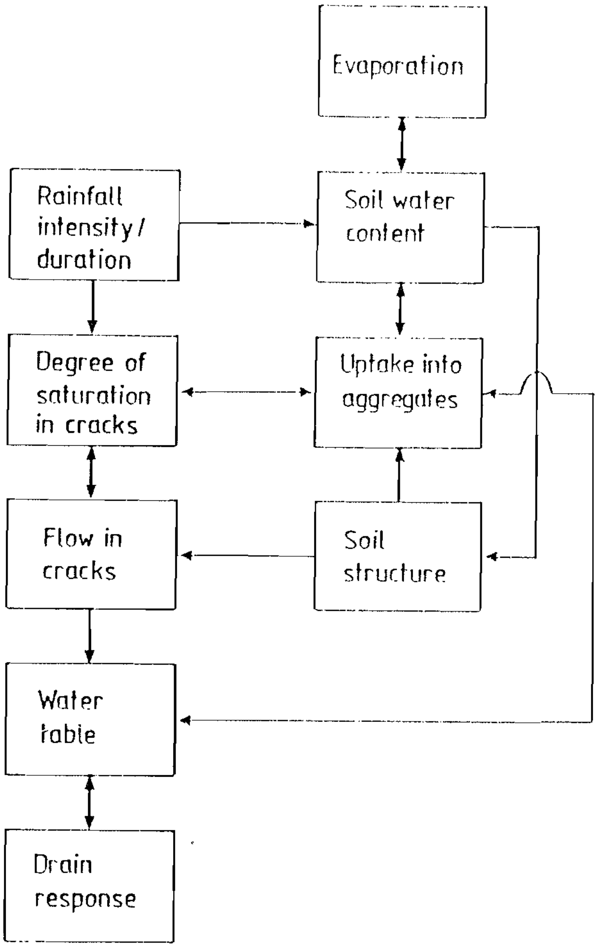


Figure 1 Flow chart of the water balance model.

where Θ and Θ_f are the current and field capacity volumetric water contents of the matrix (expressed on a whole soil basis) respectively, e_s is the stable crack porosity (i.e. structural shrinkage - Stirk, 1954), e_a is the air content of the matrix at field saturation (i.e. trapped air) and p is the shrinkage factor (i.e. the slope of the shrinkage characteristic for the soil aggregates, see Bronswijk, 1988). The value of p varies between zero for a rigid non-swelling soil and unity for aggregates that shrink normally.

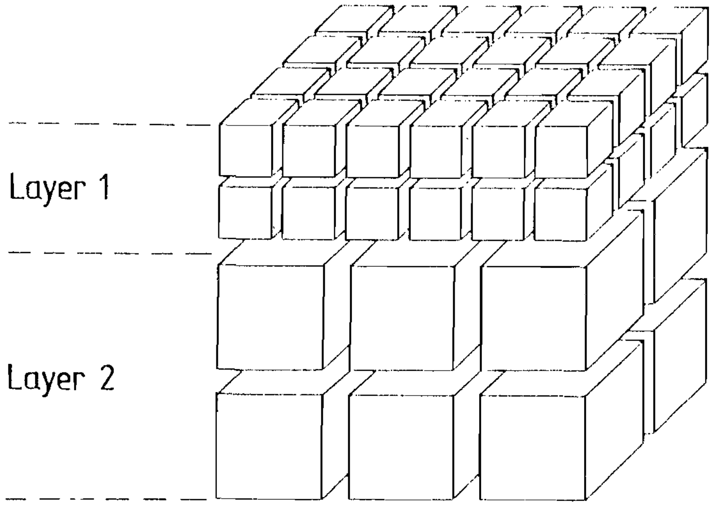


Figure 2 Soil structure assumed in the model.

Thus, the vertical component of swelling/shrinkage is neglected (i.e. layer thicknesses are constant), as it is assumed that the effects of vertical soil displacement on the soil hydrology are negligible in comparison to the effects of swelling/shrinkage in the horizontal dimensions.

Thus, if it is assumed that the aggregate width (d, ~ crack spacing) is large in relation to crack width (w), then it follows from the simple geometry (Fig.2) :

$$e_c = \frac{3\,w}{d} \tag{4}$$

and $$A_t = \frac{6}{d} \tag{5}$$

where A_t is the ped surface area per unit soil volume.

Precipitation

It is assumed that 'raindays' may be characterized by a single storm at a constant intensity (R). Irrigation is also considered in the model, with the user specifying the dates of irrigations and the amount and intensity of application on each occasion. If irrigation water is applied on a rainday, a weighted mean precipitation intensity is calculated.

Interception

A running water balance is computed for the canopy such that water is stored up to a maximum limit (the canopy interception capacity). The interception capacity is assumed to increase linearly from zero at crop emergence to a maximum value when leaf area is also at a maximum (see 'Crop development').

Precipitation which exceeds the canopy capacity becomes effective rainfall and enters the soil profile (see 'Recharge'). Canopy storage is also emptied by evaporation. The potential wet canopy evaporation rate (E_{wp}) is expressed as :

$$E_{wp} = c_t . E_p \tag{6}$$

where E_p is the potential transpiration rate calculated using a generalized Penman equation (see 'Transpiration and root water uptake') and c_t is an empirical correction factor to account for enhanced evaporation loss from a wet canopy ($c_t > 1.0$).

If the calculated value of E_{wp} is larger than the amount of water stored on the canopy (S_i), then the wet canopy evaporation is set to the canopy storage and an additional potential transpiration loss (E_t) occurs :

$$E_t = E_p - \left(\frac{S_i}{c_t}\right) \tag{7}$$

However, if canopy storage is larger than the calculated value of E_{wp} then wet canopy evaporation constitutes the total evapotranspiration loss and no additional demand is made on the soil water storage (i.e. $E_t = 0$).

Recharge

The first term of Philip's infiltration equation (Philip, 1957) is used to partition effective rain (or irrigation) falling on the soil surface into water entering aggregates and water flowing into cracks (see Fig.3). Two factors control this process, namely the rainfall intensity and the sorption capacity (I_p) of the aggregates :

$$I_p = \frac{S}{2\,t^{0.5}} \tag{8}$$

such that

$$t_p = \left(\frac{S}{2R}\right)^2 \tag{9}$$

where S is Philip's sorptivity, t is the time since the start of rainfall and t_p is the time to ponding of the soil surface. Sorptivity is assumed to be a linear function of the soil water content between field capacity and wilting point (Θ_w) :

$$S = S_w \; \{ 1 - (\frac{\Theta - \Theta_w}{\Theta_f - \Theta_w})\} \tag{10}$$

where S_w is the sorptivity at wilting point.

From equations (8) and (9) it follows that for a 24 h period :

$$\begin{array}{llll} I_m = R & ; \quad I_c = 0 & ; \quad 0 < t < t_p & \\ I_m = I_p & ; \quad I_c = R - I_p & ; \quad t_p < t < t_r & (11) \\ I_m = 0 & ; \quad I_c = 0 & ; \quad t_r < t < 24 & \end{array}$$

where I_c and I_m are the input rates to the cracks and matrix respectively and t_r is the rainfall duration given by :

$$t_r = \frac{r_{eff}}{R} \tag{12}$$

where r_{eff} is the effective rainfall amount (see 'Interception').

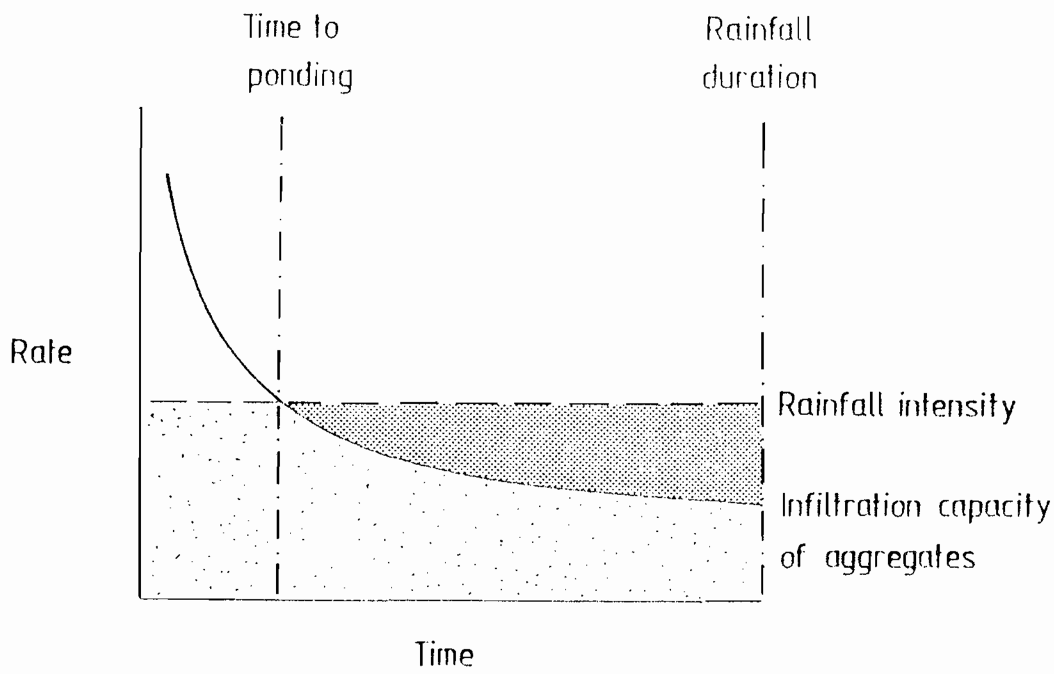


Figure 3 Partitioning of rainfall into flow of water in cracks and uptake by aggregates. Heavy dotted area indicates infiltration into cracks, light dotted area indicates uptake by aggregates.

Water in aggregates

Flow of water in aggregates is assumed negligible : peds simply act as shrinking desorbers (see 'Evaporation and root water uptake') and swelling absorbers of water. Uptake of water by aggregates may occur through the soil surface (see 'Recharge'), but also through internally wetted aggregate surfaces (i.e. water in cracks). At any given time, any number of discrete 'packets' of water may exist in the cracks within the soil profile, originating from various rain events (see 'Water in cracks'). Uptake rates are calculated separately for each packet (I_r), using a modified version of equation (8) which accounts for the fractional wetted aggregate surface area (a^*) and the fractional wetted depth in each layer (f^*) :

$$I_r = \sum_{i=1}^{i=j} (\Delta z_{(i)} \cdot f^*_{(i)}) \cdot (a^* \cdot A_{t(i)}) \cdot \left\{ \frac{S_{(i)}}{2(t - t_{c(i)})^{0.5}} \right\} \quad (13)$$

where Δz is the layer thickness, t_c is the time of first input of water into the layer and j is the number of layers. It should also be noted that we assume $a^* = 1$ for layers, or parts of layers, in which the cracks are saturated (see 'Water table position and drainage').

Water in cracks

Water in the cracks may be either mobile (i.e. above the wetting front during rainfall) or stagnant (i.e. 'old water' remaining from previous raindays). During rainfall, stagnant water is incorporated into the mobile phase as the wetting front in the cracks moves down the profile.

The flow rate of mobile water (q) is predicted as a function of crack width, porosity and degree of saturation (S_c), based on a theoretical analysis by Childs (1969, p.197) and a modification to account for flow path tortuosity and connectivity (e.g. Germann and Beven, 1981) :

$$q = (\rho g / 12\eta) \cdot w^2 \cdot e_c \cdot S_c^n \quad (14)$$

where g is the acceleration due to gravity, ρ and η are the density and viscosity of water respectively, and n is an empirical exponent termed the tortuosity factor.

If it is assumed that water flowing in a crack which is not fully saturated does so by 'bridging' across the crack, then :

$$S_c = a^* \quad (15)$$

This equality enables us to couple the rate of water uptake into aggregates with the flow of water in cracks. Using an iterative procedure known as interval halving, the program does this by determining for successive small time steps (Δt), a value of S_c which solves the water balance and thus satisfies continuity :

$$C_{(t)} = C_{(t-\Delta t)} + I_c + U - I_r \quad (16)$$

where I_r (calculated using equation (13)) refers only to water absorbed by aggregates above the wetting front, and U and C are the amount of stagnant water incorporated into the mobile phase and the amount of mobile water stored in the cracks above the wetting front respectively, given by :

$$U = q \cdot S_{c(s)} \cdot e_c \tag{17}$$

and

$$C = S_c \sum_{i=1}^{i=j} f^* \cdot \Delta z \cdot e_c \tag{18}$$

where $S_{c(s)}$ refers to the degree of saturation of the stagnant water ahead of the wetting front and j is the number of soil layers.

In this way, a new value of the fractional wetted depth for the layer in which the wetting front is located is calculated every time step :

$$f^*_{(t)} = f^*_{(t-\Delta t)} + \left(\frac{\Delta t \cdot q}{\Delta z} \right) \tag{19}$$

The water balance described by equation (16) neglects surface runoff. If the rainfall intensity exceeds the combined flow capacity of cracks and aggregates, then equation (16) cannot be solved and S_c approaches unity within the iteration loop. In this situation, S_c is set to unity and the excess water is lost as surface runoff (see 'Runoff').

The reasoning underlying equations (14) to (19) is now explained in more detail. To simplify calculations in the model, an ideal geometry is used to represent the soil structure (i.e. cubic aggregates separated by planar cracks, see 'Soil structure'). However, it is recognized that the geometry of flow paths in macroporous soils in the field is somewhat more complex. In general, cracks may be of variable thickness in the longitudinal direction (i.e. contain constrictions or 'pore necks' where aggregate surfaces are closer together). Assuming that the input rate of water at the soil surface is not sufficient to saturate the crack, water will tend to flow (at a slight suction) at the narrowest points (see Fig.4). As the input rate at the surface increases (see equation (11)), the degree of saturation in the crack will also tend to increase. Water now flows in the wider parts of the crack (at an even smaller suction) and at a faster rate. This acts as a negative feedback, regulating the degree of saturation in the cracks. An increase in crack saturation is also counter-balanced by higher uptake rates into aggregates (equation (13)). Thus, an equilibrium is established between the input rate at the surface, the change in storage within the crack, the uptake rate into aggregates and the flow rate in cracks.

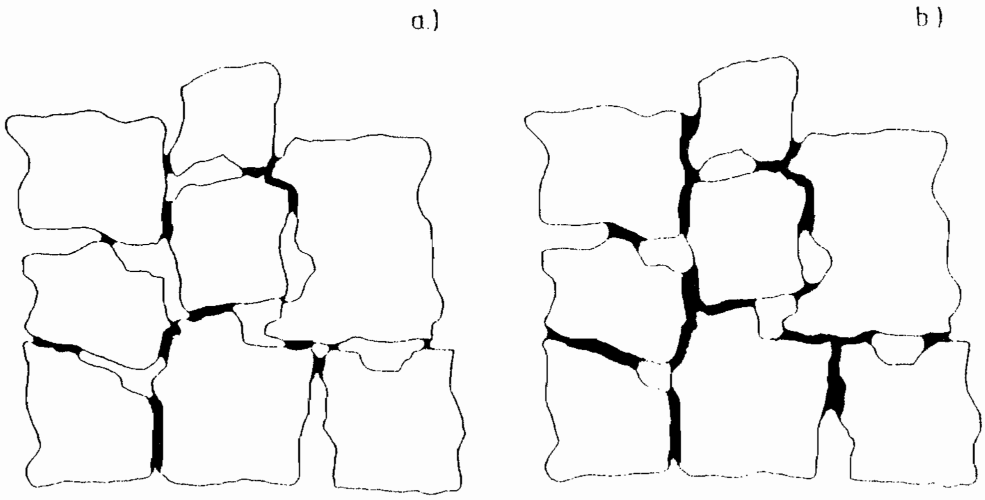


Figure 4 Flow of water in cracks (plan view) at a.) low input rates and b.) high input rates.

Water table position and drainage

The drains are assumed to respond when the soil becomes saturated above drain depth. In the model, two zones of saturation may exist in the cracks within the soil profile : a continuously fluctuating 'groundwater' table and a transient 'perched' water table. Matrix saturation is assumed not to result in drain outflow, since no true groundwater table is modelled in CRACK. Instead, excess water above field capacity is automatically lost as deep seepage (see 'Water in aggregates').

If the wetting front is not connected to the 'groundwater' table in the cracks, then the change in water table height (ΔH) is simply given by :

$$\Delta H = \frac{(- Q - I_r)\ \Delta t}{e_c} \tag{20}$$

where Q is the drain outflow rate and I_r refers only to uptake by aggregates below the groundwater table.

If the wetting front in the cracks reaches the groundwater table, then S_c is held constant and excess water generated at the interface serves to increase the height of the water table by an amount :

$$\Delta H = \frac{(I_c - Q - I_r)\ \Delta t}{e_f} \tag{21}$$

where I_r now refers to water uptake by aggregates over the entire profile depth and e_f is the fillable crack porosity given by :

$$e_f = e_c\ (1 - S_c) \tag{22}$$

If the groundwater table reaches the soil surface, the surplus water is lost as 'saturation excess' surface runoff.

The drain outflow is calculated using seepage potential theory (Youngs, 1980) :

$$Q = \frac{E}{Y} \tag{23}$$

where Y and E are the shape factor and the seepage potential respectively, given by :

$$Y = \frac{D^2}{8} \tag{24}$$

where D is the drain spacing

$$\text{and} \quad E = \sum_{z=0}^{z=H} K_z \, (H - z) \, dz \tag{25}$$

where H is the water table height above drain depth, K_z is the saturated hydraulic conductivity (varies with height z above the drain). In the model, equation (25) is solved numerically for all layers above the drain (Leeds-Harrison et al., 1986), assuming that the hydraulic conductivity in any given layer (K_i) may be expressed as a linear function of the crack porosity :

$$K_i = \frac{e_c \, . \, K_f}{e_s} \tag{26}$$

where K_f is the minimum saturated hydraulic conductivity attained when the soil matrix is fully wetted (i.e. $\Theta = \Theta_f$ and $e_c = e_s$).

If the site does not contain field drains, then an effective seepage rate is calculated from the known catchment area by assuming the site to be square in shape and bounded by imaginary ditches which penetrate to the base of the soil profile (Youngs, 1980).

A perched water table may develop during rainfall or irrigation if the precipitation intensity exceeds the combined flow capacity of cracks and aggregates (i.e. $S_c = 1$). This perched water table results in an additional seepage flow to the drains, calculated as above, but taking the position of the wetting front in the cracks as the effective drain depth. If excess water still remains to be disposed of, then it is removed by surface runoff (see following section).

Runoff

In the model, surface runoff may be generated in two ways : a 'saturation excess' runoff occurs if the groundwater table in the cracks reaches the soil surface, whilst an 'infiltration excess' runoff may occur if an infiltration throttle causes a perched water table to develop (see 'Water table position and drainage').

Crop development

A simple description of the development of an annual crop is assumed in the model (see Fig.5). A perennial crop such as grass can also be modelled by an appropriate choice of input parameter values (see p.26 and 27).

Both crop height and root depth increase at a constant rate following crop emergence up to a maximum value. Crop height is zero both before emergence and after harvest, whilst the effective 'root depth' is set to some initial minimum value in order to estimate bare soil evaporation.

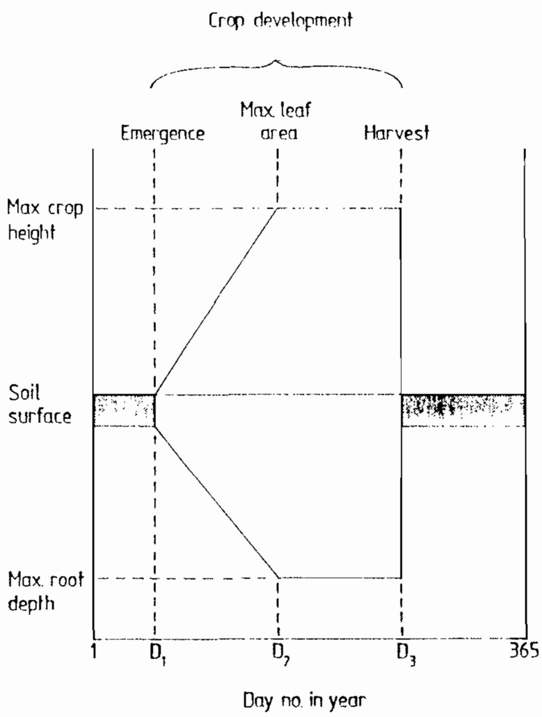


Figure 5 Development of an annual crop in the model. Shaded area represents the depth of drying of bare soil.

Transpiration and root water uptake

Potential transpiration (E_p) is calculated using a generalized form of Penman's equation with canopy (r_c) and aerodynamic resistances (r_a) made explicit :

$$\lambda E_p = \frac{\Delta (R_n - G) + (\rho_a . C_p \{ VPD/r_a \})}{\Delta + \gamma(1 + \{r_c / r_a\})} \tag{27}$$

where λ is the latent heat of vapourization, Δ is the slope of the saturated vapour pressure versus temperature curve, ρ_a and C_p are the density and specific heat capacity of air, R_n is the net radiation (estimated from sunshine hours), G is the soil heat flux (estimated as 5% of R_n), γ is the psychrometric constant, and VPD is the vapour pressure deficit.

The unstressed canopy resistance is closely related to leaf area and hence crop development. In the model, it is assumed to vary sinusoidally as a function of the number of days (D) since crop emergence :

$$r_c = (\frac{r_{max} + r_{min}}{2}) - [(\frac{r_{max} - r_{min}}{2}) . \cos \{2\pi(\frac{D - D_2}{2D^*})\}] \tag{28}$$

where r_{max} and r_{min} are the maximum and minimum values of canopy resistance (see Fig.6) and D_2 and D^* are defined in Figs.5 and 6.

The aerodynamic resistance is calculated from the logarithmic wind profile assuming that the resistances to water vapour and momentum transfer are equal :

$$r_a = [\frac{\ln \{(z^* - d_o)/z_o\}^2}{k^2 .u}] \tag{29}$$

where u is the windspeed at reference height z^* above ground level, k is von Karman's constant and d_o and z_o are the zero plane displacement height and roughness length. d_o and z_o are given as constant fractions (0.63 and 0.13 respectively) of the crop height (Monteith, 1973, pp. 88-90).

The transpiration demand E_t equals E_p if the canopy is dry. However, if intercepted water is held on the crop canopy, a proportion of the available energy is expended in evaporating this water, and the estimated potential transpiration rate is thereby reduced (see equation (7)).

Fig.7 shows how the actual transpiration loss (E_a) is calculated from the potential transpiration using the concept of a weighted stress index ($\bar{\alpha}$) (Jarvis, 1988b). The threshold value of the weighted stress index below which a reduction in transpiration rate occurs ($\bar{\alpha}_c$, see Fig.7), is termed the root adaptability factor, since effectively it allows the crop to adjust to stress in one part of the root system by increasing uptake from other parts where conditions are more favourable.

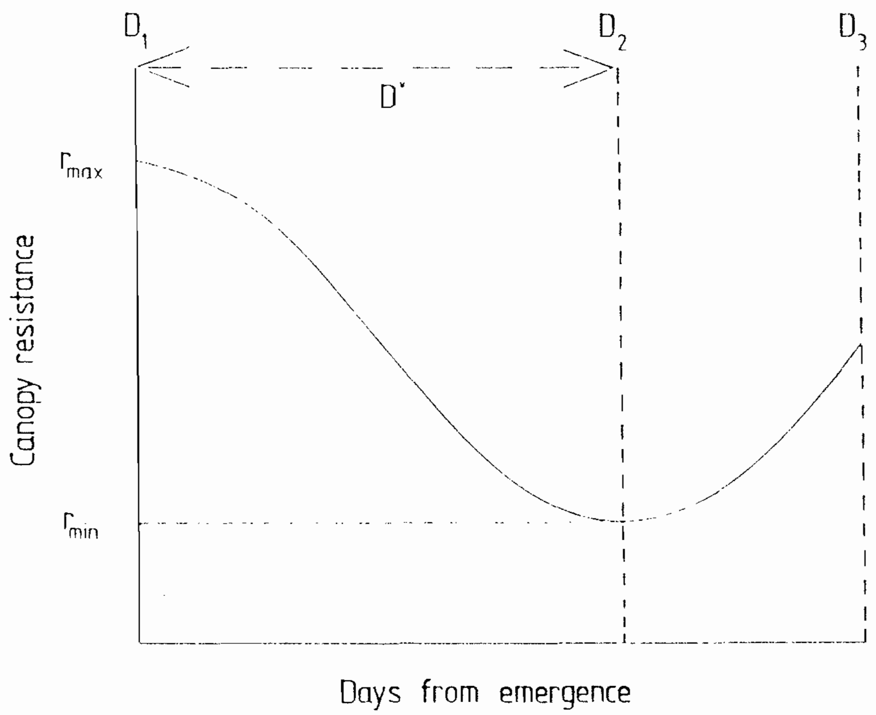


Figure 6 Canopy resistance related to crop development in the model (see Figure 5 for definition of D_1, D_2 and D_3)
[note: if $(D_3 - D_2) > (D_2 - D_1)$ then $D^* = (D_3 - D_2)$]

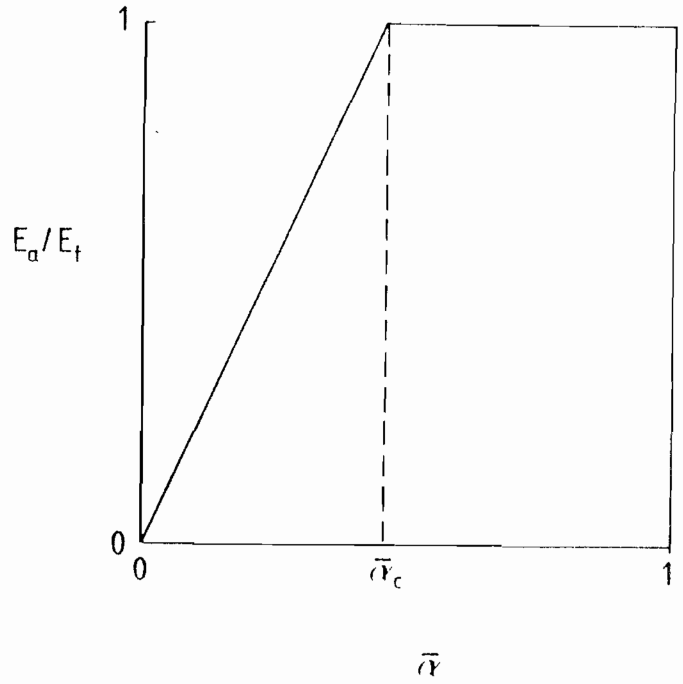


Figure 7 Actual transpiration (E_a) as a function of the potential transpiration and the weighted stress index ($\bar{\alpha}$).

The weighted stress index is calculated by combining two functions describing the distribution of roots and water content in the soil profile :

$$\bar{\alpha} = \sum_{i=1}^{i=j} R^*_i \quad . \quad \alpha_i \tag{30}$$

where j is the number of soil layers in the profile, and R^*_i and α_i are the proportion of the total root length and a water stress 'reduction factor' in layer i respectively.

The reduction factor is defined as a function of soil water content as shown in Fig.8, accounting for soil conditions that are either too wet (aeration stress, critical value Θ_{c2}) or too dry (drought stress, critical value Θ_{c1}).

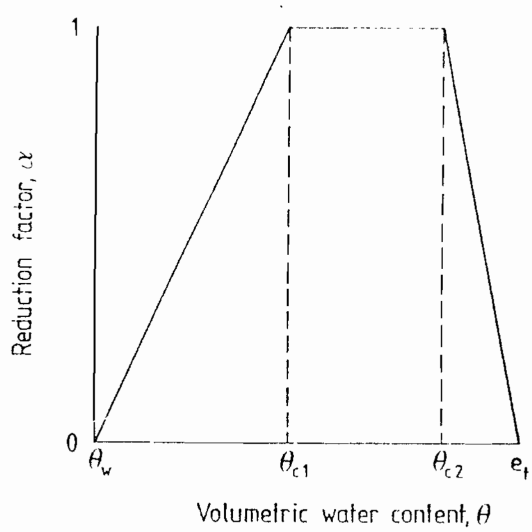


Figure 8 Water stress 'reduction factor'

Root length is assumed to be distributed logarithmically with depth (Gerwitz and Page, 1974) :

$$R^*_i = f\left(\frac{\Delta z_i}{z_r}\right) e^{-f(z_i/z_r)} \tag{31}$$

where Δz_i and z_i are the thickness and mid-point depth below the soil surface of layer i respectively, z_r is the root depth (see Fig.5) and f is an empirical root distribution parameter.

Finally, the total water uptake (E_a) is distributed within the root depth according to the weighted stress in each layer. Actual water uptake in any given layer (W_i) is therefore given by :

$$W_i = E_a \cdot \frac{\{R^*_i(\alpha_i)\}}{\bar{\alpha}} \tag{32}$$

If the surface is not cropped (i.e. before emergence or after harvest), a specified minimum 'root depth' (see Fig.5) is taken as the effective depth of drying, and potential evaporation is calculated using equation (27). The same factor for sub-optimal soil water content is used as for a cropped surface (see Fig.8), except that no reduction in evaporation is made for a soil that is too wet.

Solute transport

An option exists in CRACK to simulate the transport of solute in addition to water. The solute is assumed to be a non-reactive tracer which may be indigenous to the soil and/or applied at the soil surface in rainfall or irrigation. Two mechanisms are assumed to dominate the transport of solute in a structured soil : mass flow in mobile crack water and diffusion within aggregates (including diffusive exchange of solute with water in cracks). Mass transport of solute in cracks occurs both above the wetting front during rainfall and also in saturated layers below the groundwater table. The amount of solute transported is simply calculated from the known amount of water flowing in cracks between soil layers and the solute concentration in the crack water in each layer.

Similarly, the amount of solute leached to the drains is calculated knowing the proportion of the total drain outflow originating from each soil layer (see 'Water table position and drainage') and the solute concentration in the cracks in each layer.

Mass transport of solute into aggregates (i.e. in water absorbed by aggregates) is also considered in the model.

The aggregates are divided into segments of equal volume, and Fick's law is used to predict the rate of solute diffusion (q_s) between adjacent segments (Addiscott, 1982) :

$$q_s \quad = \quad D_o \,.\, \Theta_p \,.\, k^* \,.\, A_s \,.\, (dc/dx) \qquad (33)$$

where D_o is the diffusion coefficient in free water, k^* is the impedance factor, A_s and dc/dx are the mean cross-sectional area (per unit soil volume) and the solute concentration gradient between adjacent segments respectively, and Θ_p is the volumetric water content of the aggregates given by :

$$\Theta_p = \frac{\Theta}{1 - e_c} \tag{34}$$

Diffusive exchange of solute between the outer-most segment of the aggregates and the water-filled cracks is calculated using equation (33), but modified to account for the degree of saturation in the cracks.

The model currently assumes that solute is not taken up by the crop. Thus, soil drying due to evaporation and root water uptake increases the soil solute concentration.

INPUT PARAMETER ESTIMATION

Table 1 summarizes the input data required by CRACK. The parameters and variables have been classified into soil, crop, weather, site and solute information. Each of these groups is discussed in detail in the following sections.

Soil data

Many of the soil parameters required by the model are standard (i.e. saturated hydraulic conductivity, porosity, field capacity, wilting point). As such, some data may already be available for a particular site. For example, an extensive soils database has been collated (and also computerised) which covers very many Swedish soil profiles (e.g. Andersson and Wiklert, 1972). Other soil parameters in the model are less often measured (i.e. sorptivity) and will usually require additional experimental work. Further details on recommended measurement and estimation techniques are given below.

Total porosity should be measured in a sample which is large enough to be representative of the soil structure. The ball replacement method described by Hall et al. (1977) is useful in this context.

Field capacity and wilting point water contents may be determined by standard laboratory techniques such as tension tables and pressure plate apparatus. For most practical applications, field capacity can be defined as the equilibrium volumetric water content at a given tension in the range 0.002 to 0.01 MPa.

DATA GROUP	PARAMETER OR VARIABLE	SYMBOL (eqn no.)[fig.no.]	COMMENTS AND ESTIMATION TECHNIQUES
SOIL	Total porosity	e_t (1)	Measured in the field (bulk soil value)
	Initial soil water contents	-	Known.
	Field capacity	Θ_f (2,3,10)	Fully swollen water content (cracks empty)(= tension of 0.02-0.1 MPa). Measured.
	Wilting point	Θ_w (10)[8]	Water content at tension of 1.5 MPa Measured.
	Critical soil water contents	Θ_{c1},Θ_{c2} [8]	Root water uptake affected by drought and oxygen stress. Literature values.
	Stable crack porosity	e_s (2,26)[9]	Crack porosity of fully swollen soil. Measured.
	Hydraulic conductivity	K_f (26)[9]	Saturated (fully swollen soil). Measured.
	Slope of shrinkage characteristic	p (2,3)[10]	Mean value between field capacity and wilting point. Measured.
	Sorptivity	S_w (10)[11]	Measured at (or extrapolated to) wilting point.
	Tortuosity factor	n (14)	Controls flow of water in cracks Calibrated.
	Crack spacing	d (4,5)[2]	= aggregate size. Measured/estimated.
WEATHER	Sunshine hours	(27)	Driving variable in calculation of evapotranspiration (Penman). Measured.
	Wind speed	(29)	"
	Air temperature	(27)	"
	Vapour pressure	(27)	"
	Daily rainfall	[13]	Driving variable.
	Rainfall intensity	R (9,12)[13]	Measured/estimated.

SITE	Site latitude	-	Known.
	Drain depth	(25)	Known.
	Drain spacing	D (24)	Known.
	Site catchment area	-	If site has no field drains. Known/estimated.
CROP	Maximum crop height	[5]	Known/estimated.
	Initial and Maximum root depths	[5]	Measured/estimated.
	Root distribution	f (31)	Measured/literature values
	Emergence and harvest dates	D_1, D_3 [5,6]	Known.
	Date on which leaf area is a maximum	D_2 (28)[5,6]	Measured/estimated.
	Maximum and Minimum surface resistance	r_{max},r_{min} (28)[6]	Sinusoidal variation between these limits. Literature values.
	Adaptability factor	α_c [7]	Crop adjustment to water stress. Calibrated.
	Canopy interception capacity	-	At maximum crop leaf area Literature values.
	Ratio wet canopy to dry canopy evaporation	c_t (6,7)	Literature value
SOLUTE	Diffusion coefficient in free water	D_o (33)	Literature values.
	Impedance factor	k^* (33)	Literature/estimated/calibrated.
	Solute concentrations in irrigation & rainfall	-	Known.
	Initial soil solute concentrations	-	Known.

Table 1 Summary of input parameters/variables required by the model

However, the use of tension tables may lead to problems in estimating field capacity in highly swelling and shrinking soils, since it is difficult to define the volume of the sample if it has shrunk away from the core wall. Field data (e.g. Reid and Parkinson, 1987) may then provide more reliable estimates of field capacity.

Stable crack porosity is defined as the volume fraction of water released between saturation and field capacity in a fully swollen soil. It may be estimated using the laboratory techniques discussed above, although more representative results may be obtained on larger samples.

Saturated hydraulic conductivity may be measured in standard constant or falling head apparatus in the laboratory, or instead estimated from infiltration measurements in the field. However, problems may be encountered with both of these techniques.

The standard size of core sample (both length and diameter) used for laboratory measurements of hydraulic conductivity is often too small to be representative of the scale of natural soil structure. The values obtained are usually highly variable, and probably not representative. The true field value may be either overestimated (due to truncation of otherwise dead-end large pores) or underestimated (due to inadequate sampling of large pores).

Double-ring infiltrometers at least sample a larger soil volume. However, problems may occur with lateral flow, particularly if the soil is layered. Improved field techniques to estimate saturated hydraulic conductivity for large undisturbed samples are described by Bouma (1982).

It should also be remembered that the saturated hydraulic conductivity is not considered as a constant in the model. The user is required to input a value for the minimum attainable saturated hydraulic conductivity (i.e. with the soil matrix fully wetted).

Leeds-Harrison et al. (1986) have described a laboratory technique which avoids many of the problems discussed above, giving reliable estimates of saturated hydraulic conductivity for large undisturbed soil monoliths (see Fig.9).

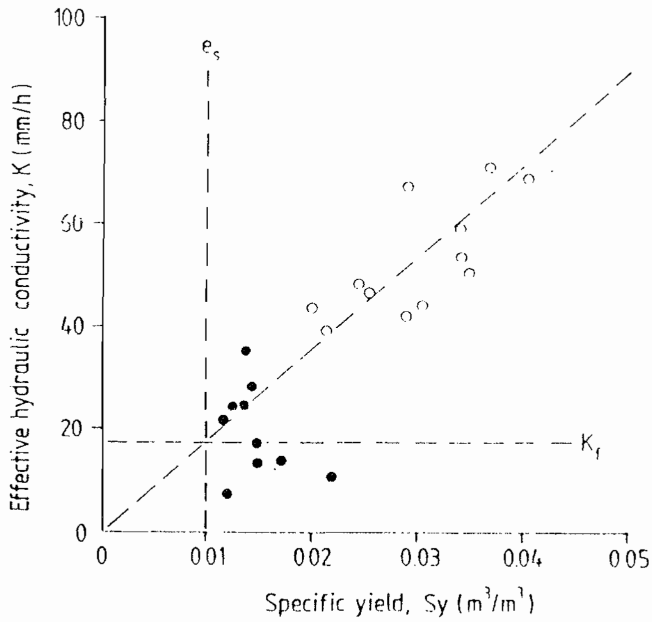


Figure 9 Hydraulic conductivity as a function of specific yield (Evesham series clay soil, 0-20 cm depth ; ○ 1 day pre-wetting, ● 21 days pre-wetting ; e_s and K_f are defined in text). Re-drawn from Leeds-Harrison and Shipway (1985).

One advantage with this approach is that a relationship may be determined between the effective hydraulic conductivity and the specific yield (i.e. drainable porosity). Estimates of the stable crack porosity (e_s) and the minimum attainable saturated hydraulic conductivity (K_f) are obtained if the soil monolith is fully saturated before making the measurements (see Fig.9).

<u>Critical soil water contents</u> are required as model input. These are expressed as : the percentage depletion of soil water storage from saturation (i.e. a drought induced reduction in water uptake), and the critical soil air content (i.e. an aeration stress effect on water uptake). It is probably easiest to take both these values from the literature. For example, a critical aeration level of 10-12% is often quoted for unstructured sand, whereas a lower figure (1-6%) is perhaps more appropriate for well-structured clay (Feddes et al., 1978).

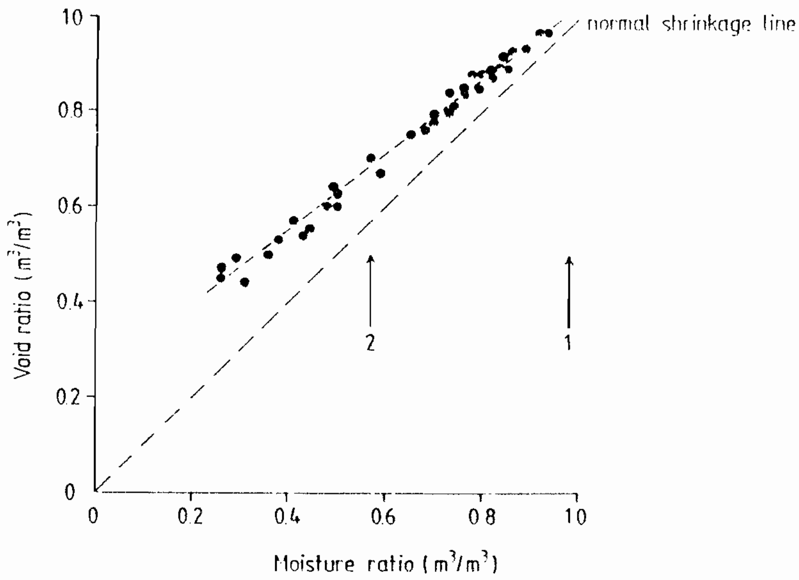


Figure 10 Shrinkage characteristic (Evesham series clay soil, 10 cm depth, 1 = saturation, 2 = wilting point ; slope of the characteristic (p) = 0.8).

<u>Shrinkage characteristics</u> may be determined in the laboratory on natural soil aggregates coated with saran resin (Brasher et al., 1966). The user should specify an average slope of the shrinkage characteristic (= shrinkage factor) for the range of available water (i.e. between field capacity and wilting point)(see Fig.10).

<u>Sorptivity</u> is easily measured in the field using a tension infiltrometer (Clothier and White, 1981)(see Fig.11). An estimate is required of the aggregate (i.e. matrix) sorptivity at wilting point. This does not necessarily mean, of course, that the measurements must be made at wilting point. It is possible to extrapolate from measurements made at any known water content, if it is assumed that sorptivity is a linear function of the soil water content between field capacity and wilting point.

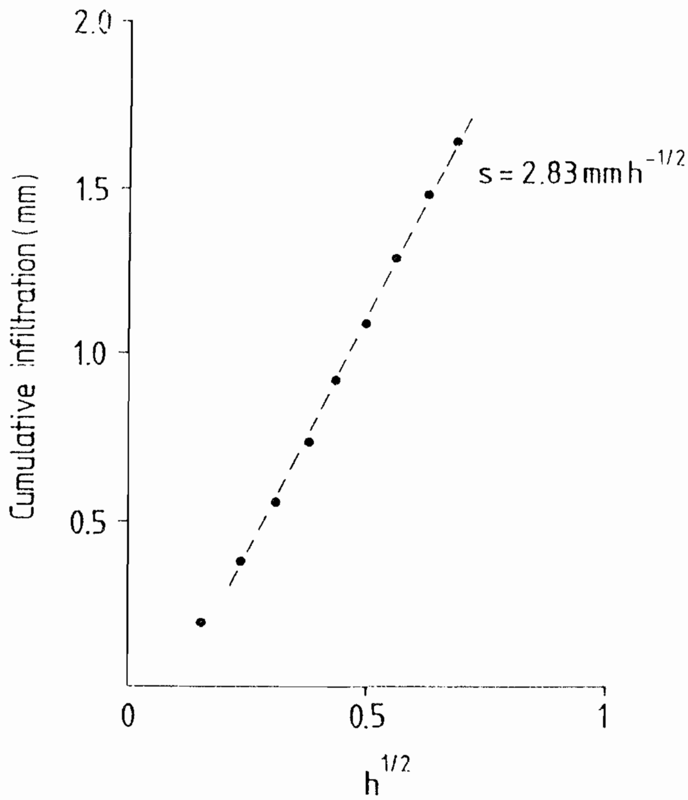


Figure 11 Sorptivity (S) derived from a plot of cumulative infiltration vs. the square root of time (tension infiltrometer measurements in Evesham series clay). Re-drawn from Jarvis et al. (1987).

Tortuosity factor. It is not possible to directly measure this model parameter. Instead, it is recommended that a value be determined by calibrating model predictions against suitable experimental data (e.g. measurements of soil water content or drain outflow). If a long time-series of measured data is available, then a small sub-set (preferably a major re-wetting period) should be employed for this purpose. The optimized value which is obtained should subsequently be tested by running the model with the remaining data set. The current, rather limited, experience suggests that the value of this parameter may lie between 1.5 and 2.5 for well-structured clay soils.

Crack spacing is particularly difficult to define in the field, although a number of techniques are available. These include image analysis (Scott et al., 1986), the plaster of paris method (FitzPatrick et al., 1985), and dry sieving (Spoor and Godwin, 1984). Whichever technique is chosen, it is important to obtain reasonable estimates of crack spacing for each soil horizon, since it is known that model predictions are particularly sensitive to this parameter (Jarvis and Leeds-Harrison, 1987a).

Image analysis is perhaps the most objective, quantitative method although it is generally too expensive and time-consuming for most routine modelling applications. Dry sieving may be the best method for tilled layers, though not really appropriate for undisturbed subsoils. Both these methods will give frequency distributions of aggregate sizes (or crack spacings), whereas a single value (for each layer) is required as model input. The geometric mean value may then be the best approximation.

It is probably better to correctly identify differences in soil structure between horizons within the soil profile in a semi-quantitative, or even qualitative way, rather than expending a great amount of time and effort to obtain accurate estimates of the absolute values of this model parameter at perhaps only one or two depths. It is therefore recommended that a full soil profile description be made at the site of interest, with particular attention paid to soil structure description. Representative values of crack spacing for each designated horizon could be based on a combination of this soil profile description and perhaps the use of the plaster of paris method (FitzPatrick et al., 1985), a rapid way of highlighting major soil structural features.

Crop data

Emergence and harvest dates are required as input in the model. With regard to the former, the date at which 50% of the crop has emerged is often used. If a perennial crop (i.e. grass) is to be simulated, then the user should specify emergence and harvest dates which lie outside the simulation period (otherwise bare soil evaporation will be calculated). The user should also be aware of the fact that, in the model, it is not too easy to account for the development pattern of a perennial crop which is harvested more than once during the year (i.e. an intensively managed grass ley). Sequential simulation of each growth period is possible, but tedious to handle.

The date on which leaf area is a maximum is also needed. This may be roughly estimated from general knowledge, or alternatively observations of ground cover or leaf area index may be used.

The maximum crop height may be estimated from simple field observations or measurements. It should be noted that the height of a perennial crop is assumed to be constant (i.e. this value).

Initial and maximum root depths. The role of the initial root depth is twofold. Firstly, it defines the starting depth for root growth of an annual crop (i.e. seed placement depth). Secondly, it defines the depth of soil drying due to bare soil evaporation. If a perennial crop is to be simulated, it is very important that the user ensures that the initial root depth and the maximum root depth are the same value in order that a zero root penetration rate is calculated.

The maximum root depth may be obtained in several ways. Direct observation in a profile pit is perhaps the simplest and is also fairly reliable. If more detailed, quantitative data on root development is available (e.g. observation tubes, rhizotrons, or core samples) then this is to be preferred. However, it is not likely that this information will be generally available, and it is not worth the time or effort to collect such data solely for routine model applications.

A useful technique to infer effective root depths from frequent soil water content measurements (e.g. by neutron probe) is described by McGowan (1974)(see Fig.12). In addition to the maximum root depth, an effective emergence date may also be estimated by extrapolating backwards, knowing the average root growth rate. Care should be taken if the soil water content data set used to determine these parameters is also being used to validate the model. In this situation, it should be split into two sub-sets, one for calibration and one for testing.

Root distribution is assumed logarithmic with depth. The user must supply a value for the percentage of roots within the top 25% of the root depth. This may be obtained by direct field measurements or observations or a suitable value chosen from the literature (e.g. Gerwitz and Page, 1974).

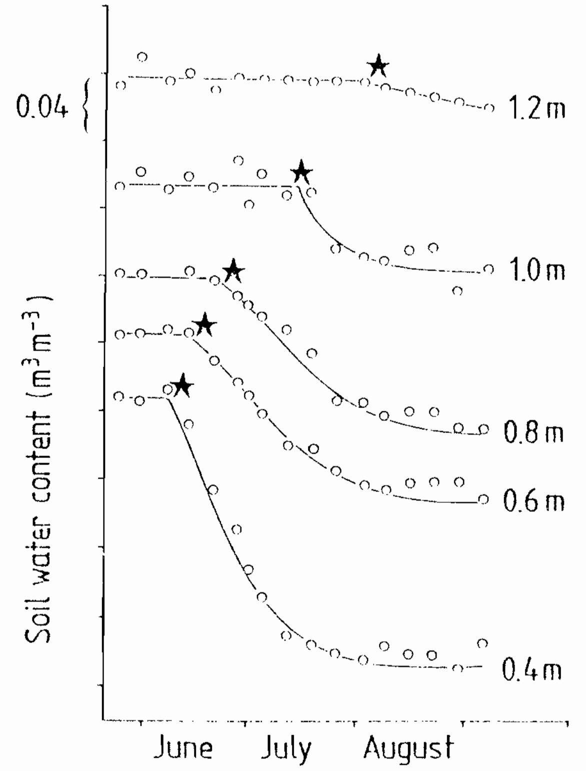


Figure 12 Soil water content as a function of time under a potato crop (Cottenham series sandy loam ; figures indicate measurement depth ; stars indicate arrival of the 'rooting front'). Re-drawn from Parker et al. (1988).

<u>Maximum and minimum crop surface resistance</u> values should be obtained from the literature, unless measurements of stomatal resistance and leaf area are available for the site in question. The user should check that the values used refer to unstressed canopy resistance (i.e. with optimum water supply and nutrition).

The adaptability factor is a measure of the crops ability to adjust its pattern of root water uptake in response to stress. It cannot be easily measured, so again a value must be determined by optimizing model predictions against field data. The somewhat limited experience to date is that the value of this parameter may vary depending on prior stress treatment. For pre-stressed crops, it may lie between 0.1 and 0.3, but a value much closer to unity may be more appropriate for well-watered crops.

The canopy interception capacity is well documented for many crops. Values generally lie between 1 and 3 mm for most agricultural crops. For an annual crop, a value appropriate to a fully developed canopy should be given.

The ratio between wet and dry canopy evaporation strongly depends on surface roughness (i.e. crop height). Values close to 1.0 may be reasonable for some short crops, whereas larger values (perhaps up to 2.0) may be more appropriate for taller row crops and trees. It should be noted that no adjustment of this parameter is made to account for the increase in height of an annual crop through the year.

Site data

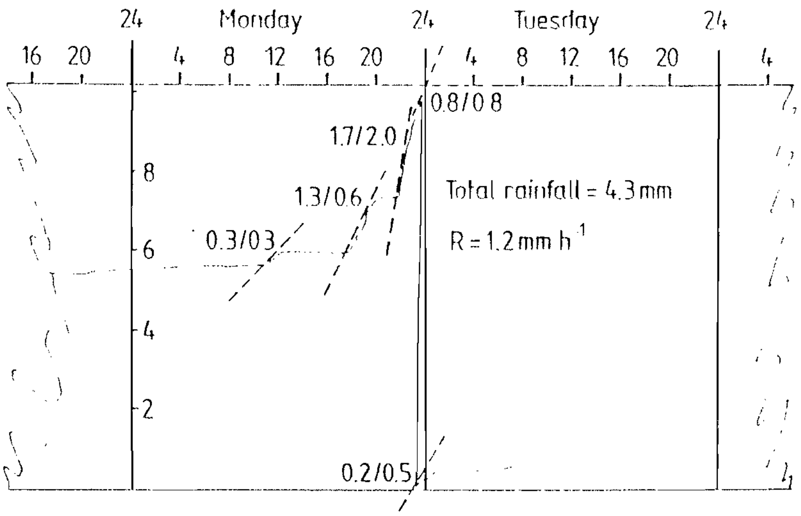
Site latitude must be given.

Drain depth and spacing are input to the model if the site has field drains. If it does not, the user must instead enter a value for the effective site catchment area.

Weather data

Meteorological data is required on a daily basis as driving variables to the model (sunshine hours, air temperature, vapour pressure, wind speed and rainfall amount). Generally, this data will be obtained from the nearest synoptic weather station.

Rainfall intensity. A single value of rainfall intensity is assumed to characterize any rainday. Some weather stations (particularly those located at Research Institutes, Universities, and some airports) maintain continuously recording automatic rain gauges. If the weather station is sited close to the field site, a weighted mean rainfall intensity for each rainday may be derived from these records (see Fig.13 for an example).



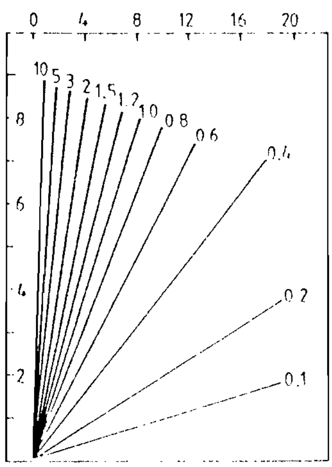


Figure 13 Estimation of mean daily rainfall intensity from a chart- recording automatic rain gauge. Upper diagram is an example of a chart record from Ultuna, Uppsala, with the rainfall amounts given for individual storms (first figure) and the corresponding intensities (after slash - second figure) estimated by using the template shown in the lower diagram.

note: the mean intensity was calculated as follows :
[0.3 (0.3/4.3)] + [0.6 (1.3/4.3)] + ...

Alternatively, if such measured data is not available, an option exists within the model to substitute an average rainfall intensity for the (unknown) actual value for that day. A sinusoidal variation within the year is assumed, and values for the minimum and maximum rainfall intensity and the date on which the minimum occurs are input.

Irrigation dates, amounts and intensities, if any, must also be given.

Solute data (optional)

The number of segments constituting the aggregates (i.e. to calculate intra-aggregate solute diffusion) should be at least ten to reduce numerical computation errors to an acceptable level (Addiscott, 1982).

Diffusion coefficient in free water. Values for many solutes and tracers of interest are well established and may be obtained from the literature (e.g. Nye and Tinker, 1977).

The impedance factor is assumed constant in the model. A typical value may be selected from the literature (Nye and Tinker, 1977), or alternatively, this parameter may be treated as a calibration or fitting parameter in the model validation procedure.

Initial concentration in the soil solution must be given for each layer, together with single values (which may be different) for the solute concentration in rainfall and irrigation.

OPERATION OF THE MODEL

Computer equipment

The model may be run either on a VAX computer or on IBM PC, XT, AT (or fully compatible) with 640 kB internal memory. If you wish to run the model on a personal computer, it is strongly recommended that you use a PC AT (80286 processer) with hard disk and numeric co-processer. If you do not, file handling will be difficult and the run-time is likely to be prohibitively long. Even with this equipment, the model may take up to 2 hours to simulate one year (the ratio CPU time to simulated real time is approx. $2 \cdot 10^{-4}$). The user should also be aware that if solute transport is to be simulated, run-times may double.

Preparation

The first stage is to prepare a weather data file which covers the period you wish to simulate (see Appendix 1 for an example). The user is afforded some flexibility, since both the first and last days of the simulation period are specified elsewhere (see 'Running the model' - these may be varied with each model run) and need not exactly correspond to the first and last days of the weather data file. The file may also be prepared in free format, although the order of variables and their units are fixed. You should note that reading from left to right, the columns are (see also Appendix 1) :

- the date as a six digit number (year, month, day).
- air temperature in °C.
- vapour pressure in mbars.
- sunshine hours.
- wind speed in ms^{-1} at a reference height of 2 m.
- rainfall amount in mm.
- rainfall intensity in mmh^{-1} (optional).

Once you have prepared the weather data file, then you may run the model.

Running the model

For the first simulation at any given site, you should run the model interactively. If you are running the PC version simply type :

> crack

or if it is the VAX version type :

$ run crack

You must now answer a number of questions concerning choice of options, input and output filenames and parameter input values. To help you answer questions concerning parameter input values, you are given some information concerning the correct units to use. For those parameters which require a value for each layer in the profile, you should separate the values with a comma. A complete example of a model run in this interactive mode, together with additional comments, is given in Appendix 2.

During this initial simulation, a log file (CRACK.LOG) is created which stores your answers to the questions. If you wish to change any parameter value, you simply edit this log file. It is then convenient to re-run the model from the edited log file, which may also be renamed (e.g. you may want to include a site descriptor). For example, if CRACK.LOG has been renamed to SILSOE.IN (SILSOE refers to the site name, IN stands for input), then to run the model on the PC simply type :

> crack <silsoe.in

or to run in batch on the VAX, rename the log file SILSOE.COM (i.e. command file) and type :
$ submit silsoe

You may also edit the log file to include comments on any line (e.g. a name to remind the user which parameter the value(s) refer to, and their units). Parameter values must be separated from comments by exclamation marks. Examples of files prepared in this way are given in Appendix 3.

Numerical considerations
The user must specify values for both the time step, and the layer thicknesses in the soil profile, bearing in mind that numerical instabilities will occur if too large values are chosen. A basic time step of the order of 0.1 h is appropriate if only the water balance is to be simulated. A smaller time step (0.01-0.02 h) will probably be necessary to ensure numerical stability if solute transport is also to be simulated. For days with no rainfall or irrigation, the specified time step is multiplied by a factor of ten, in order to speed up execution times.

Layer thicknesses should also depend on morphological properties of the soil profile of interest, as well as on the numerical considerations already discussed.

Output
Two basic output files are produced by a model run, the first containing data on the components of the soil water balance and the second soil water contents in each layer (see Appendices 4 and 5 respectively). A third output file is produced if the solute transport option is being used (see Appendix 6).

In all three output files, the date is given in the first column as a six digit number enclosed by apostrophes. This output format enables the user of CRACK to input results of model simulations to a graphics package named PGRA. This package is user-friendly (with complete help library) and was specifically developed to handle time-series data. Enquiries concerning PGRA should be addressed to Dr. Per-Erik Jansson, Department of Soil Sciences, Swedish University of Agricultural Sciences (specify either PC or VAX version).

MODEL LIMITATIONS

CRACK is a specialized model, and as such has rather well defined limits of applicability. These should be recognized and clearly understood by the model user. The most important of these limitations are now discussed.

Matrix flow

Water movement is not considered in the soil matrix. This considerably simplifies the mathematical treatment of flow interactions between the two domains (cracks/aggregates), but it also means that the model can only be applied to soils of low matrix hydraulic conductivity (i.e. of fine texture). To date, the model has only been applied to soils with a clay content of at least 50% throughout the profile. However, the actual limit should be somewhat lower than this, perhaps 30-40% clay content.

Structural stability

The model assumes that the flow region consists of an active (i.e. dynamic) inter-connecting network of cracks and fissures. This implies that the soil structure is stable throughout wetting and drying cycles (i.e. no deflocculation, crusting or capping). This, in turn, means that the model may not work well in soils of high silt content, or sodium saturated clays. As yet, however, there is no real evidence which would either confirm or deny this argument.

Soil freezing

Since the model takes no account of soil heat flow, it cannot be applied to winter periods characterized by snow and frost.

Artesian water

The model does not consider the possibility of a supply of water to the soil profile by upward flow of groundwater under pressure. Thus, it should not be applied to those depressional areas within the landscape which experience this phenomena.

FUTURE DEVELOPMENT

This section indicates some future developments of the model which may increase the scope of possible applications.

Additional subroutines/options

A number of additional subroutines are planned including :

- a sub-model of crop growth which would improve upon the simple description currently in the model.
- options to predict transport and transformations of specified solutes (e.g. nitrate, pesticides).
- a sub-model to characterize the effects of soil tillage and compaction by agricultural traffic.
- a sub-model to predict the effects of soil structure and soil strength on root penetration and water uptake.

Link to other models

A second-generation simplified version of CRACK will be developed which retains the conceptual framework of the full model. This would be in a format suitable for linking with other models. For example, a link is planned to the SOIL model of Jansson and Halldin (1979), a comprehensive model of water and heat flow in a layered soil profile.

This will enable model users to evaluate the effects of macropores in a wider range of soil types, sites and climates (e.g. in coarser textured soils than clay, texturally layered soil profiles (e.g. clay over sand), depressional water-receiving sites and winter climates in which snow-pack and soil freezing are important phenomena).

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Appendix 1 Weather data file

Units as stated

(1) Date
(2) Air temperature (^{o}C)
(3) Vapour pressure (mbars)
(4) Sunshine hours
(5) Wind speed ($m\ s^{-1}$)
(6) Rainfall (mm)
(7) Rainfall intensity ($mm\ h^{-1}$)

(1)	(2)	(3)	(4)	(5)	(6)	(7)
850401	12.4	12.8	.4	7.0	.0	.0
850402	9.9	9.6	6.9	4.5	.0	.0
850403	15.4	12.1	2.3	4.4	.0	.0
850404	11.6	10.6	.5	3.7	.0	.0
850405	10.8	10.1	1.0	2.6	.0	.0
850406	9.1	8.9	6.1	3.0	.0	.0
850407	7.6	9.6	1.2	4.9	2.5	2.3
850408	8.9	10.0	2.1	3.6	.0	.0
850409	9.0	10.1	7.4	3.0	.0	.0
850410	8.8	9.1	5.1	2.7	3.2	3.1
850411	6.3	9.0	.7	8.9	.6	2.5
850412	7.5	10.2	5.6	6.1	.5	2.5
850413	8.0	9.4	6.3	6.2	.0	.0
850414	6.9	9.9	3.3	5.2	.0	.0
850415	9.6	8.4	4.2	3.1	.0	.0
850416	13.2	11.5	8.8	2.1	.0	.0
850417	11.8	10.4	.4	.6	.0	.0
850418	12.3	11.7	5.9	1.3	.0	.0
850419	14.4	10.6	9.2	4.0	.0	.0
850420	6.6	6.6	1.9	1.4	.5	2.5
850421	7.0	8.7	4.3	3.9	.0	.0
850422	8.5	8.4	9.2	5.5	.0	.0
850423	5.4	6.7	6.9	3.9	.0	.0
850424	5.8	6.0	12.1	2.2	.0	.0
850425	6.8	7.7	.4	1.6	.0	.0
850426	6.7	5.8	6.6	4.2	.0	.0
850427	8.6	7.8	1.2	4.5	1.4	1.5
850428	4.9	4.9	6.3	2.4	2.6	.4
850429	4.9	7.9	.0	1.8	1.7	5.4
850430	11.3	12.0	3.8	3.8	.0	.0

Appendix 2 Interactive model run with comments

Numbers in parentheses refer to comments

ENTER NAME OF FILE CONTAINING WEATHER DATA : w.dat

DOES YOUR FILE CONTAIN RAINFALL INTENSITY DATA ? : y

ENTER SITE LATITUDE (in radians) : 0.92

ENTER START DATE : 850401 (1)

ENTER END DATE : 850430 (2)

ENTER NUMBER OF IRRIGATIONS : 2

ENTER DATE OF IRRIGATION : 850406 (3)

ENTER DATE OF IRRIGATION : 850419

ENTER IRRIGATION AMOUNTS (mm) : 20.0,30.0

ENTER IRRIGATION INTENSITIES (mm/h) : 4.0,5.0

ENTER TIME INTERVAL (h) : 0.1

ENTER NUMBER OF SOIL LAYERS : 5 (4)

ENTER THICKNESS OF EACH LAYER (m) : 0.2,0.2,0.2,0.2,0.2 (5)

DOES YOUR SITE CONTAIN FIELD DRAINS ? : y

ENTER DRAIN DEPTH (m) : 1.0 (6)

ENTER DRAIN SPACING (m) : 10.0

ENTER OUTPUT FILENAME (for soil water balance) : out1.dat

ENTER OUTPUT FILENAME (for soil water contents) : out2.dat

ENTER SOIL WATER CONTENT IN EACH LAYER (%) : 42.5,44.0,45.3,46.0,47.0 (7)

ENTER TOTAL POROSITY IN EACH LAYER (%) : 50,50,50,50

Incorrect no. of layers in your answer (8)

ENTER TOTAL POROSITY IN EACH LAYER (%) : 50,50,50,50,50

ENTER FIELD CAPACITY IN EACH LAYER (%) : 47,47,47,47,47

ENTER STABLE CRACK POROSITY IN EACH LAYER (%) : 4,3,2,1,1

The values you have specified exceed total porosity (9)

ENTER TOTAL POROSITY IN EACH LAYER (%) : 50,50,50,50,50

ENTER FIELD CAPACITY IN EACH LAYER (%) : 47,47,47,47,47

ENTER STABLE CRACK POROSITY IN EACH LAYER (%) : 2,2,2,2,2 (10)

ENTER WILTING POINT IN EACH LAYER (%) : 25,25,25,25,25

ENTER CRACK SPACING IN EACH LAYER (m) : 0.1,0.2,0.3,0.4,0.4

ENTER SHRINKAGE FACTOR IN EACH LAYER (0 to 1) : 0.0,0.5,0.8,1.0,1.0

ENTER INITIAL DEPTH TO WATER TABLE (m) : 1.2

The value you have specified is too large (11)

ENTER INITIAL DEPTH TO WATER TABLE (m) : 0.9

ENTER TORTUOSITY FACTOR : 2.0

ENTER PED SORPTIVITY (at wilting point)(mm/h^0.5) : 3.0 (12)

ENTER MINIMUM SATURATED HYDRAULIC CONDUCTIVITY (mm/h) : 40.0 (13)

ENTER CRITICAL DEPLETION OF AVAILABLE SOIL WATER (%) : 50.0

ENTER CRITICAL SOIL AIR CONTENT (%) : 5.0 (14)

ENTER DATE OF EMERGENCE :850420

ENTER DATE OF MAXIMUM LEAF AREA : 850710

ENTER DATE OF HARVEST : 850921

ENTER INITIAL ROOT DEPTH (m) : 0.1

ENTER MAXIMUM ROOT DEPTH (m) : 0.8 (15)

ENTER PERCENTAGE OF ROOTS IN TOP 25% OF ROOT DEPTH : 65

ENTER ROOT ADAPTABILITY FACTOR (0 to 1) : 0.2

ENTER MAXIMUM CROP HEIGHT (m) : 0.7

ENTER MAXIMUM CROP SURFACE RESISTANCE (s/m) : 200.0

ENTER MINIMUM CROP SURFACE RESISTANCE (s/m) : 50.0

ENTER INTERCEPTION CAPACITY (mm)(max. leaf area) : 2.0

ENTER CORRECTION FACTOR FOR WET CANOPY EVAPORATION : 1.5

DO YOU WANT TO SIMULATE SOLUTE TRANSPORT ? n

NOTES :

(1) Dates are expressed as a six digit number (year, month and day).

(2) Both start and end dates must lie within the range of dates in your weather data file (although they need not necessarily be the first and last days in the file). The maximum simulation period possible at present is one year.

(3) Irrigation dates need not lie within the current simulation period (e.g. start and/or end dates may be changed in later simulations thereby including irrigation events).

(4) Must not exceed twenty.

(5) Layer thicknesses need not be equal, as here.

(6) Must not exceed total profile depth.

(7) Known initial soil water contents.

(8) User error ! Values for only four layers were specified. If you make such an error on any question, it will be repeated until a correct answer (i.e. number of values) is given.

(9) User error ! The total porosity of the surface soil layer (50%) is exceeded by the combined total of the field capacity soil water content (47%) and the stable crack porosity (4%). Input questions are repeated until correct answers are given.

(10) Acceptable answers this time round (1% trapped air content in the matrix implied)

(11) User error ! The depth to the water table specified here exceeds the total profile depth (= 1.0 m). The question is repeated.

(12) Defines sorptivity-soil water content relationship. Note that if either wilting point or field capacity water content values (in the surface soil layer) are subsequently changed, then the slope of this relationship is also changed.

(13) Defines hydraulic conductivity-crack porosity relationship. Note that if stable crack porosity (in the surface soil layer) is subsequently changed, then the slope of this relationship is also changed.

(14) The user should ensure that the value specified here does not result in 'overlapping' (i.e. you must ensure that $\Theta_{c1} < \Theta_{c2}$, see Fig.8) since no internal check for this is made in the program.

(15) For perennial crops, it is important to ensure that initial and maximum root depths are equal.

Appendix 3 Parameter input files (edited log files)

a.) log file to interactive model run shown in Appendix 2, edited to delete mistakes and include comments concerning parameters.

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! INPUT/OUTPUT FILENAMES, WEATHER/SITE DATA, NUMERICAL CONSIDERATIONS !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
w.dat                    ! Weather data file
y                        ! Rainfall intensity data ?
0.92                     ! Site latitude (radians)
850401                   ! Start date of simulation
850430                   ! End date of simulation
2                        ! No. of irrigations
850406                   ! Date of irrigation
850419                   !       "
20,30                    ! Irrigation amounts (mm)
4,5                      ! Irrigation intensities (mm/h)
0.1                      ! Time interval (h)
5                        ! No. of soil layers
0.2,0.2,0.2,0.2,0.2      ! Layer thickness (m)
y                        ! Field drains ?
1.0                      ! Drain depth (m)
10.0                     ! Drain spacing (m)
out1.dat                 ! Output filename (soil water balance)
out2.dat                 ! Output filename (soil water contents)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!           SOIL DATA                                                 !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
42.5,44.0,45.3,46.0,47.0      ! Initial soil water content (%)
50,50,50,50,50                ! Total porosity (%)
47,47,47,47,47                ! Field capacity (%)
2,2,2,2,2                     ! Stable crack porosity (%)
25,25,25,25,25                ! Wilting point (%)
0.1,0.2,0.3,0.4,0.4           ! Crack spacing (m)
0,0.5,0.8,1.0,1.0             ! Shrinkage characteristic
0.9                           ! Initial depth to water table (m)
2                             ! Tortuosity factor
3                             ! Aggregate sorptivity (mm/h^0.5)
40                            ! Saturated hydraulic conductivity (mm/h)
50                            ! Critical depletion of available water (%)
5                             ! Critical soil air content (%)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          CROP DATA                                                  !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
850420              ! Emergence date
850710              ! Date of maximum leaf area
850921              ! Harvest date
0.1                 ! Initial root depth (m)
0.8                 ! Maximum root depth (m)
65                  ! Root distribution (% in top 25% of root depth)
0.2                 ! Adaptability factor
0.7                 ! Maximum crop height (m)
200                 ! Maximum crop surface resistance (s/m)
50                  ! Minimum crop surface resistance (s/m)
2                   ! Interception capacity (maximum)(mm)
1.5                 ! Correction factor (evaporation of intercepted water)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
n      ! Solute transport ?                                           !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

b.) Parameter file which also simulates solute transport. The file is based on Appendix 3a with two further edits (time interval and end date of simulation have been changed)

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! INPUT/OUTPUT FILENAMES, WEATHER/SITE DATA, NUMERICAL CONSIDERATIONS !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
w.dat                  ! Weather data file
y                      ! Rainfall intensity data ?
0.92                   ! Site latitude (radians)
850401                 ! Start date of simulation
850420                 ! End date of simulation
2                      ! No. of irrigations
850406                 ! Date of irrigation
850419                 !       "
20,30                  ! Irrigation amounts (mm)
4,5                    ! Irrigation intensities (mm/h)
0.02                   ! Time interval (h)
5                      ! No. of soil layers
0.2,0.2,0.2,0.2,0.2    ! Layer thickness (m)
y                      ! Field drains ?
1.0                    ! Drain depth (m)
10.0                   ! Drain spacing (m)
out3.dat               ! Output filename (soil water balance)
out4.dat               ! Output filename (soil water contents)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!         SOIL DATA                                                    !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
42.5,44.0,45.3,46.0,47.0       ! Initial soil water content (%)
50,50,50,50,50                 ! Total porosity (%)
47,47,47,47,47                 ! Field capacity (%)
2,2,2,2,2                      ! Stable crack porosity (%)
25,25,25,25,25                 ! Wilting point (%)
0.1,0.2,0.3,0.4,0.4            ! Crack spacing (m)
0,0.5,0.8,1.0,1.0              ! Shrinkage characteristic
0.9                            ! Initial depth to water table (m)
2                              ! Tortuosity factor
3                      ! Aggregate sorptivity (mm/h^0.5)
40                     ! Saturated hydraulic conductivity (mm/h)
50                     ! Critical depletion of available water (%)
5                      ! Critical soil air content (%)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!         CROP DATA                                                    !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
850420          ! Emergence date
850710          ! Date of maximum leaf area
850921          ! Harvest date
0.1             ! Initial root depth (m)
0.8             ! Maximum root depth (m)
65              ! Root distribution (% in top 25% of root depth)
0.2             ! Adaptability factor
0.7             ! Maximum crop height (m)
200             ! Maximum crop surface resistance (s/m)
50              ! Minimum crop surface resistance (s/m)
2               ! Interception capacity (maximum)(mm)
1.5             ! Correction factor (evaporation of intercepted water)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!         SOLUTE DATA                                                  !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
y                      ! Solute transport ?
out5.dat               ! Output filename (solute information)
0.0                    ! Solute concentration in rainfall (kg/m3)
1.0                    ! Solute concentration in irrigation (kg/m3)
0.0,0.0,0.0,0.0,0.0    ! Initial soil solute concentration (kg/m3)
10                     ! No. of segments per soil layer
2.0E-09                ! Diffusion coefficient in free water (m2/s)
0.4                    ! Impedance factor
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

c.) Parameter file derived from Appendix 3b. The file has been edited to make the site undrained and unirrigated. Note also that the time interval has been further reduced and we are now simulating movement of indigeneous solute rather than transport of solute applied in irrigation water.

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! INPUT/OUTPUT FILENAMES, WEATHER/SITE DATA, NUMERICAL CONSIDERATIONS !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
w.dat                    ! Weather data file
y                        ! Rainfall intensity data ?
0.92                     ! Site latitude (radians)
850401                   ! Start date of simulation
850420                   ! End date of simulation
0                        ! No. of irrigations
0.005                    ! Time interval (h)
5                        ! No. of soil layers
0.2,0.2,0.2,0.2,0.2      ! Layer thickness (m)
n                        ! Field drains ?
5.0                      ! Site catchment area (ha)
out3.dat                 ! Output filename (soil water balance)
out4.dat                 ! Output filename (soil water contents)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          SOIL DATA                                                     !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
42.5,44.0,45.3,46.0,47.0         ! Initial soil water content (%)
50,50,50,50,50                   ! Total porosity (%)
47,47,47,47,47                   ! Field capacity (%)
2,2,2,2,2                        ! Stable crack porosity (%)
25,25,25,25,25                   ! Wilting point (%)
0.1,0.2,0.3,0.4,0.4              ! Crack spacing (m)
0,0.5,0.8,1.0,1.0                ! Shrinkage characteristic
0.9                      ! Initial depth to water table (m)
2                        ! Tortuosity factor
3                        ! Aggregate sorptivity (mm/h^0.5)
40                       ! Saturated hydraulic conductivity (mm/h)
50                       ! Critical depletion of available water (%)
5                        ! Critical soil air content (%)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          CROP DATA                                                     !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
850420           ! Emergence date
850710           ! Date of maximum leaf area
850921           ! Harvest date
0.1              ! Initial root depth (m)
0.8              ! Maximum root depth (m)
65               ! Root distribution (% in top 25% of root depth)
0.2              ! Adaptability factor
0.7              ! Maximum crop height (m)
200              ! Maximum crop surface resistance (s/m)
50               ! Minimum crop surface resistance (s/m)
2                ! Interception capacity (maximum)(mm)
1.5              ! Correction factor (evaporation of intercepted water)
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
!          SOLUTE DATA                                                   !
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
y                        ! Solute transport ?
out5.dat                 ! Output filename (solute information)
0.0                      ! Solute concentration in rainfall (kg/m3)
0.1,0.1,0.1,0.1,0.1      ! Initial soil solute concentration (kg/m3)
10                       ! No. of segments per soil layer
2.0E-09                  ! Diffusion coefficient in free water (m2/s)
0.4                      ! Impedance factor
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

Appendix 4 Output file (soil water balance)

All units are in millimetres, except where stated.

(1) Date
(2) Water table depth (m)
(3) Drain outflow
(4) Surface runoff
(5) Deep seepage
(6) Actual evaporation (cumulative)
(7) Potential transpiration (cumulative)
(8) Actual evaporation
(9) Potential transpiration
(10) Canopy storage
(11) Soil water deficit
(12) Precipitation

(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)
'850401'	-.9168	.3	.0	.0	1.4	1.4	1.4	1.4	.0	40.2	.0
'850402'	-.9287	.2	.0	.0	3.7	3.7	2.3	2.3	.0	42.7	.0
'850403'	-.9376	.2	.0	.0	6.0	6.0	2.3	2.3	.0	45.1	.0
'850404'	-.9446	.1	.0	.0	7.5	7.5	1.5	1.5	.0	46.7	.0
'850405'	-.9501	.1	.0	.0	8.8	8.8	1.4	1.4	.0	48.2	.0
'850406'	-.7011	4.5	.0	.0	10.9	10.9	2.0	2.0	.0	34.8	20.0
'850407'	-.8022	2.3	.0	.0	12.1	12.1	1.2	1.2	.0	35.8	2.5
'850408'	-.8588	1.1	.0	.0	13.5	13.5	1.4	1.4	.0	38.3	.0
'850409'	-.8901	.6	.0	.0	15.5	15.5	2.1	2.1	.0	41.0	.0
'850410'	-.9093	.4	.0	.0	17.4	17.4	1.9	1.9	.0	40.0	3.2
'850411'	-.9228	.3	.0	.0	18.6	18.6	1.2	1.2	.0	40.9	.6
'850412'	-.9328	.2	.0	.0	20.3	20.3	1.6	1.6	.0	42.3	.5
'850413'	-.9408	.2	.0	.0	22.4	22.4	2.2	2.2	.0	44.6	.0
'850414'	-.9471	.1	.0	.0	23.8	23.8	1.3	1.3	.0	46.1	.0
'850415'	-.9522	.1	.0	.0	25.9	25.9	2.2	2.2	.0	48.3	.0
'850416'	-.9564	.1	.0	.0	28.7	28.7	2.8	2.8	.0	51.2	.0
'850417'	-.9599	.1	.0	.0	30.0	30.0	1.2	1.2	.0	52.5	.0
'850418'	-.9629	.1	.0	.0	32.1	32.1	2.2	2.2	.0	54.7	.0
'850419'	-.6272	8.0	.0	.0	35.9	35.9	3.7	3.7	.0	36.4	30.0
'850420'	-.7814	3.2	.0	.0	37.3	37.3	1.5	1.5	.0	40.5	.5
'850421'	-.8484	1.3	.0	.0	39.2	39.2	1.9	1.9	.0	43.7	.0
'850422'	-.8839	.7	.0	.0	40.3	40.3	1.2	1.2	.0	45.6	.0
'850423'	-.9060	.4	.0	.0	41.3	41.3	1.0	1.0	.0	47.0	.0
'850424'	-.9209	.3	.0	.0	42.9	42.9	1.6	1.6	.0	48.9	.0
'850425'	-.9318	.2	.0	.0	43.7	43.7	.8	.8	.0	49.9	.0
'850426'	-.9400	.2	.0	.0	44.9	44.9	1.2	1.2	.0	51.3	.0
'850427'	-.9462	.1	.0	.0	45.8	45.7	.9	.9	.0	50.9	1.4
'850428'	-.9513	.1	.0	.0	47.1	46.9	1.3	1.2	.0	49.7	2.6
'850429'	-.9555	.1	.0	.0	47.5	47.3	.4	.3	.0	48.5	1.7
'850430'	-.9591	.1	.0	.0	48.3	48.1	.8	.8	.0	49.4	.0

Note : This output file was produced from a model run with the parameter file shown in Appendix 3a.

Appendix 5 Output file (soil water contents)

Units are m^3 m^{-3}

(1) Date
(2) Soil water content (top layer)
(3) Soil water content (bottom layer)

(1)	(2)				(3)
'850401'	.418	.440	.453	.460	.478
'850402'	.407	.440	.453	.460	.477
'850403'	.395	.440	.453	.460	.476
'850404'	.388	.440	.453	.460	.476
'850405'	.381	.440	.453	.460	.475
'850406'	.409	.444	.455	.478	.490
'850407'	.415	.444	.455	.467	.490
'850408'	.408	.444	.455	.467	.484
'850409'	.398	.444	.455	.467	.481
'850410'	.404	.444	.455	.467	.479
'850411'	.401	.444	.455	.467	.478
'850412'	.396	.444	.455	.467	.477
'850413'	.385	.444	.455	.467	.476
'850414'	.378	.444	.455	.467	.475
'850415'	.367	.444	.455	.467	.475
'850416'	.353	.444	.455	.467	.474
'850417'	.347	.444	.455	.467	.474
'850418'	.336	.444	.455	.467	.474
'850419'	.378	.448	.464	.487	.490
'850420'	.374	.448	.464	.471	.490
'850421'	.364	.448	.464	.470	.485
'850422'	.359	.448	.464	.470	.482
'850423'	.354	.448	.464	.470	.479
'850424'	.346	.448	.464	.470	.478
'850425'	.342	.448	.464	.470	.477
'850426'	.336	.448	.464	.470	.476
'850427'	.338	.448	.464	.470	.475
'850428'	.345	.448	.464	.470	.475
'850429'	.351	.448	.464	.470	.474
'850430'	.347	.448	.464	.470	.474

Note : This output file was produced from a model run with the parameter file shown in Appendix 3a.

Appendix 6 Output file (solute transport)

Units as stated

(1) Date

Top line, reading from left

Total profile solute content (kg ha^{-1})
Solute in drainage (cumulative)(kg ha^{-1})
Solute in surface runoff (cumulative)(kg ha^{-1})
Solute concentration in drainage (kg m^{-3})

Second line, reading from left

Solute concentration in soil layers (kg m^{-3})
(top layer .... bottom layer)

(1)

```
'850401'    .00     .00     .00  .0000
   .0000  .0000  .0000  .0000  .0000
'850402'    .00     .00     .00  .0000
   .0000  .0000  .0000  .0000  .0000
'850403'    .00     .00     .00  .0000
   .0000  .0000  .0000  .0000  .0000
'850404'    .00     .00     .00  .0000
   .0000  .0000  .0000  .0000  .0000
'850405'    .00     .00     .00  .0000
   .0000  .0000  .0000  .0000  .0000
'850406' 190.95    8.99     .00  .2045
   .1228  .0237  .0153  .0362  .0212
'850407' 188,63   11.31     .00  .1021
   .1209  .0237  .0153  .0332  .0226
'850408' 187.80   12.14     .00  .0763
   .1230  .0237  .0153  .0332  .0220
'850409' 187.40   12.54     .00  .0638
   .1261  .0237  .0153  .0332  .0217
'850410' 187.18   12.76     .00  .0564
   .1241  .0237  .0153  .0332  .0216
'850411' 187.04   12.90     .00  .0513
   .1250  .0237  .0153  .0332  .0215
'850412' 186.94   13.00     .00  .0475
   .1268  .0237  .0153  .0332  .0214
'850413' 186.87   13.07     .00  .0446
   .1304  .0237  .0153  .0332  .0214
'850414' 186.82   13.12     .00  .0423
   .1327  .0237  .0153  .0332  .0213
'850415' 186.78   13.17     .00  .0404
   .1366  .0237  .0153  .0332  .0213
'850416' 186.74   13.20     .00  .0388
   .1420  .0237  .0153  .0332  .0213
'850417' 186.72   13.22     .00  .0374
   .1445  .0237  .0153  .0332  .0213
'850418' 186.69   13.25     .00  .0362
   .1491  .0237  .0153  .0332  .0213
'850419' 464.71   35.15     .00  .2782
   .3158  .0597  .0616  .0698  .0471
'850420' 459.72   40.14     .00  .1589
   .3198  .0597  .0616  .0652  .0487
```

Note : This output file was produced from a model run with the parameter file shown in Appendix 3b.

Förteckning över utgivna häften i publikationsserien.

SVERIGES LANTBRUKSUNIVERSITET, UPPSALA. INSTITUTIONEN FÖR MARKVETENSKAP. AVDELNINGEN FÖR LANTBRUKETS HYDROTEKNIK. RAPPORTER.

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111 Berglund, G. m fl. 1978. Resultat av 1977 års fältförsök avseende täckdikning, övrig grundförbättring och bevattning. 98 s.

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