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NOTA 210

CALCULATION OF UPTAKE OF NUTRIENTS AND WATER BY A ROOT SYSTEM

door

P. DE WILLIGEN

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CONTENTS

1. Introduction	2
2. Microscopic model of uptake of nutrients and water	3
2.1. Basic assumptions	3
2.2. Nutrients	3
2.3. Water	8
3. Description of uptake in a macroscopic model	10
3.1. Nutrients	10
3.2. Water	11
4. Programs	14
5. Examples	15
5.1. Water uptake	15
5.2. Nutrient uptake	18
6. Literature	21
Appendices	
Appendix I. Calculation of the nutrient uptake by a single root in a zero-sink situation	23
Appendix II. Numerical solution of radial flow of water to a plant root	42
Appendix III. Calculation of uptake of a nutrient by a root system	67
Appendix IV. Calculation of water uptake by a root system	71

1. INTRODUCTION

Microscopic models on nutrient and water transport in the soil and on uptake by the roots deal with gradients in the immediate vicinity of a single root, i.e. with transport distances of a few millimeters or less. Most of such models only consider transport in a horizontal direction, transport being described in a fundamental way using Fick's and Darcy's laws.

In macroscopic models (like crop growth models), on the other hand, the scale is of the order of 10 cm or more and interest is focused on uptake behaviour of a root system rather than that of a single root. Usually transport in vertical direction is considered only, and fluxes of water are calculated approximately, except where interest is in dynamics of water flow per se.

Ideally, the description of uptake by a root system in a macroscopic model should be based on the description of the uptake of a microscopic model. More often than not, however, the macroscopic uptake models (implicitly) lump effects of physical and physiological properties of soil and roots into one or two parameters, of which it is often difficult to comprehend how they quantitatively relate to the microscopic properties they supposedly embrace.

The first goal of this report is to discuss how results of uptake models on a microscopic scale can lead to a description of uptake on a macroscopic scale consistent with the former. A second goal is to present a documentation on the computer programs pertaining to the models discussed.

2. MICROSCOPIC MODEL OF UPTAKE OF NUTRIENTS AND WATER

2.1. *Basic assumptions*

For the microscopic model we start by considering a vertical cylindrical root. The root is situated within a cylinder of soil. Over the outer boundary of this cylinder no transport will take place. Such a root can be thought of as belonging to a set of uniformly distributed roots all equally active and of the same length.

The uptake rate is assumed to be constant and independent of the nutrient concentration (water content or matric potential in case of water uptake) as long as the latter exceeds a certain limiting value. This approach is different from that of other workers in this field (Nye and Tinker, 1977; Barber, 1984) who put most emphasis on the uptake-determining role of the concentration.

Whenever the concentration (water content, matric potential) at the root surface reaches its limiting value the uptake rate equals the rate of arrival of the nutrient (water) at the root surface, i.e. the concentration (water content) there will be maintained at the limiting value. In case of the important nutrients N and K the limiting value can be safely set at zero.

2.2 *Nutrients*

Analytical solutions

The system described in the foregoing paragraph can be formulated mathematically by a partial differential equation, describing transport by massflow and diffusion in a hollow cylinder, together with initial and boundary conditions. The boundary condition at the inner cylinder (the root) is either that of constant uptake or of zero-concentration.

De Willigen and van Noordwijk (1987) presented an analytical solution when uptake is constant and the initial concentration is uniform. It reads in dimensionless units (Table 1 explains the symbols):

TABLE 1. List of symbols.

Symbol	Name	Dimension	Dimensionless symbol
R_0	root radius	cm	-
D	diffusion coefficient	cm^2/day	-
T	time	day	$t = DT/R_0$
T_c	period of	day	t_c
$T_{c,\max}$	maximum T_c	day	$t_{c,\max}$
R	radial coordinate	cm	$r = R/R_0$
R_1	radius soil cylinder	cm	$\rho = R_1/R_0$
H	root length	cm	$\eta = H/R_0$
S	available amount of nutrient	mg/cm^3	$s = S/S_i$
S_i	initial value of S	mg/cm^3	
A	uptake rate	$\text{mg}/(\text{cm}^2 \cdot \text{day})$	$\omega = -\rho^2 \theta \beta / (2\phi \eta)$
ϕ	supply/demand parameter	-	$\phi = DS_i / (AR_0)$
C_i	initial nutrient concentration	mg/ml	-
C	nutrient concentration	mg/ml	$c = C/C_i$
θ_i	initial watercontent	ml/cm^3	-
θ	water content	ml/cm^3	-
K_a	adsorption constant	ml/cm^3	-
$\theta \beta$	buffer capacity	ml/cm^3	$\beta = (K_a + \theta) / \theta$
U_1	flow of water over the root surface	cm/day	-
U_2	flow of water from bulk soil to root surface		-
E	transpiration rate	cm/day	-
V	flux of water	cm/day	$2\nu = RV/D$
P	pressure head	cm	
D_w	diffusivity	cm^2/day	
K	conductivity	cm/day	
Φ	matric flux potential	cm^2/day	
Φ_{rs}	matric flux potential at root surface	cm^2/day	

$$c = \frac{(\rho^2-1)(\nu+1)r^{(2\nu)}}{\rho^{2\nu+2}-1} + \quad (1a)$$

$$\omega \left[\frac{2(\nu+1)r^{2\nu}}{\rho^{2\nu+2}-1} \frac{t}{\theta\beta} + \frac{r^{2\nu}(r^2-\rho^2)}{\rho^{2\nu+2}-1} + \frac{\rho^2(\rho^{2\nu}-r^{2\nu})}{2\nu(\rho^{2\nu+2}-1)} + \right. \\ \left. \frac{\rho^2(\rho^{2\nu}-1)r^{2\nu}(\nu+1)}{2\nu(\rho^{2\nu+2}-1)^2} + \frac{r^{2\nu}(\nu+1)(1-\rho^{2\nu+4})}{(2\nu+4)(\rho^{2\nu+2}-1)^2} \right] + \quad (1b)$$

$$(\omega-2\nu)r^\nu\pi \sum_{n=1}^{\infty} \frac{J_{\nu+1}(\alpha_n)J_{\nu+1}(\rho\alpha_n)}{\alpha_n} F_\nu(r, \alpha_n) e^{\frac{-\alpha_n^2 t}{\theta\beta}} + \quad (1c)$$

$$\frac{2\nu r^\nu\pi}{\rho^{\nu+1}} \sum_{n=1}^{\infty} \frac{J_{\nu+1}^2(\alpha_n)}{\alpha_n} F_\nu(r, \alpha_n) e^{\frac{-\alpha_n^2 t}{\theta\beta}} \quad (1d)$$

with:

$$F_\nu(r, \alpha_n) = \frac{Y_{\nu+1}(\rho\alpha_n)J_\nu(r\alpha_n) - Y_\nu(r\alpha_n)J_{\nu+1}(\rho\alpha_n)}{J_{\nu+1}^2(\alpha_n) - J_{\nu+1}^2(\rho\alpha_n)}$$

and α_n is the n-th root of:

$$Y_{\nu+1}(\alpha)J_{\nu+1}(\rho\alpha) - J_{\nu+1}(\alpha)Y_{\nu+1}(\rho\alpha) = 0$$

Where $J_\nu(x)$, $Y_\nu(x)$ denote the Bessel function of the first kind, order ν and argument x and the modified Bessel function of the first kind order ν and argument x respectively. Eventually the series part (1c-d) will vanish and a steady-rate situation, where concentration is a linear function of time, will develop given by (1a-1b). The uptake potential of the system can be characterized by a characteristic time constant t_u , called the period of unconstrained uptake, denoting the period during which the concentration at the root surface exceeds zero. If the concentration at the root surface reaches its limiting zero-value in the steady-rate situation, at time $t = t_u$, the concentration profile can be given by:

$$c = \omega \left[\frac{r^{2\nu+2}}{2(\rho^{2\nu+2}-1)} - \frac{r^{2\nu}(\nu+\rho^{2\nu+2})}{2\nu(\rho^{2\nu+2}-1)} + \frac{\rho^{2\nu+2}}{2\nu(\rho^{2\nu+2}-1)} \right] \quad (2)$$

If after $t = t_u$ the concentration at the root surface is constant (zero), i.e. the root behaves as a zero-sink, the concentration distribution for $t > t_u$ is given by (De Willigen and Van Noordwijk in prep.):

$$c = \frac{-2\pi\omega(\nu+1)}{\rho^{2\nu+2}-1} \sum_{n=0}^{\infty} \frac{J_{\nu}(\alpha_n)J_{\nu+1}(\alpha_n)}{J_{\nu}^2(\alpha_n) - J_{\nu+1}^2(\rho\alpha_n)} \frac{r^{\nu}C_{\nu}(r\alpha_n)}{\alpha_n^2} e^{\frac{-\alpha_n^2(t-t_u)}{\theta\beta}}, \quad (3)$$

where

$$C_{\nu}(r\alpha) = Y_{\nu}(r\alpha)J_{\nu+1}(\rho\alpha) - J_{\nu}(r\alpha)Y_{\nu+1}(\rho\alpha)$$

and α_n now is the n -th root of $C_{\nu}(\alpha) = 0$.

From (3) the uptake rate can be derived as the gradient of the concentration c at the root surface (where $r=1$):

$$\omega_t = \left(\frac{\partial c}{\partial r} \right)_{r=1} = \frac{-4(\nu+1)\omega}{\rho^{2\nu+2}-1} \sum_{n=0}^{\infty} \frac{J_{\nu+1}^2(\rho\alpha)}{\alpha^2(J_{\nu}^2(\alpha) - J_{\nu+1}^2(\rho\alpha))} e^{\frac{-\alpha_n^2(t-t_u)}{\theta\beta}} \quad (4)$$

From (4) the time-integrated uptake after the period of unconstrained uptake is found as:

$$\int_{t_u}^t \omega_t dt = \frac{-4(\nu+1)\omega\theta\beta}{\rho^{2\nu+2}-1} \sum_{n=0}^{\infty} \frac{J_{\nu+1}^2(\rho\alpha)}{\alpha^2(J_{\nu}^2(\alpha) - J_{\nu+1}^2(\rho\alpha))} \{1 - e^{\frac{-\alpha_n^2(t-t_u)}{\theta\beta}}\} \quad (5)$$

It now appears (De Willigen and Van Noordwijk 1987) that (4) can be approximated very well by a much simpler equation viz. a steady-rate equation like (2), but with time-dependent uptake rate ω_t , which is given by:

$$\omega_t = \omega e^{-\frac{t}{\theta\beta G(\rho, \nu)}}, \quad (6)$$

A consequence of the assumption of the concentration being given by (2) with ω_t instead of ω is that the former is proportional to the average concentration:

$$\omega_t = -\frac{(\rho^2-1)\bar{c}}{2G(\rho, \nu)}, \quad (7)$$

where the function $G(\rho, \nu)$ is given by:

$$G(\rho, \nu) = \frac{1}{2(\nu+1)} \left[\frac{1-\rho^2}{2} + \frac{\rho^2(\rho^{2\nu}-1)}{2\nu} + \frac{\rho^2(\rho^{2\nu}-1)(\nu+1)}{2\nu(\rho^{2\nu+2}-1)} + \frac{(1-\rho^{2\nu+4})(\nu+1)}{(2\nu+4)(\rho^{2\nu+2}-1)} \right]$$

and c denotes the average concentration in the soil solution. The above solutions (i.e. (3), (4), (5) and the approximation (6)) pertain to the situation where a steady-rate concentration profile (2) has developed before the concentration at the root surface reaches zero. When the concentration at the root surface drops to zero before the steady-rate situation has been reached - thus before the terms (1c) and (1d) can be neglected - it is assumed that the root behaves as a zero-sink from the beginning. The exact solution for the concentration is now given by (De Willigen and Van Noordwijk, unpublished):

$$c = -\pi \sum_{n=0}^{\infty} \frac{2\nu J_{\nu}^2(\alpha_n) - \alpha \rho^{\nu+1} J_{\nu}(\alpha_n) J_{\nu+1}(\alpha_n)}{J_{\nu}^2(\alpha_n) - J_{\nu+1}^2(\rho \alpha_n)} \frac{r^{\nu} C_{\nu}(r \alpha_n)}{\rho^{\nu+1} \alpha_n} e^{-\frac{\alpha_n^2 t}{\theta \beta}}, \quad (8)$$

and that for uptake by :

$$\omega_t = \left(\frac{\partial c}{\partial r} \right)_{r=1} = -2 \sum_{n=0}^{\infty} \frac{2\nu J_{\nu}(\alpha) J_{\nu+1}(\rho \alpha) - \alpha \rho^{\nu+1} J_{\nu+1}^2(\rho \alpha)}{\alpha (J_{\nu}^2(\alpha) - J_{\nu+1}^2(\rho \alpha))} e^{-\frac{\alpha_n^2 t}{\theta \beta}} \quad (9)$$

whereas the time-integrated uptake now is given by:

$$\int_0^t \omega_t dt = -2\theta\beta \sum_{n=0}^{\infty} \frac{2\nu J_{\nu}(\alpha) J_{\nu+1}(\rho \alpha) - \alpha \rho^{\nu+1} J_{\nu+1}^2(\rho \alpha)}{\alpha^2 (J_{\nu}^2(\alpha) - J_{\nu+1}^2(\rho \alpha))} \{1 - e^{-\frac{\alpha_n^2 t}{\theta \beta}}\} \quad (10)$$

Here it also appeared that the the complicated expression for uptake (9) can be very well approximated by an equation like (7).

Figure 1 shows the cumulative uptake in the zero-sink situation for the exact solutions and the approximation. Details about the calculation procedure are found in Appendix I. The approximation is shown to be quite good, so it will be used in formulating uptake in the macroscopic model to be discussed in section 3.1.

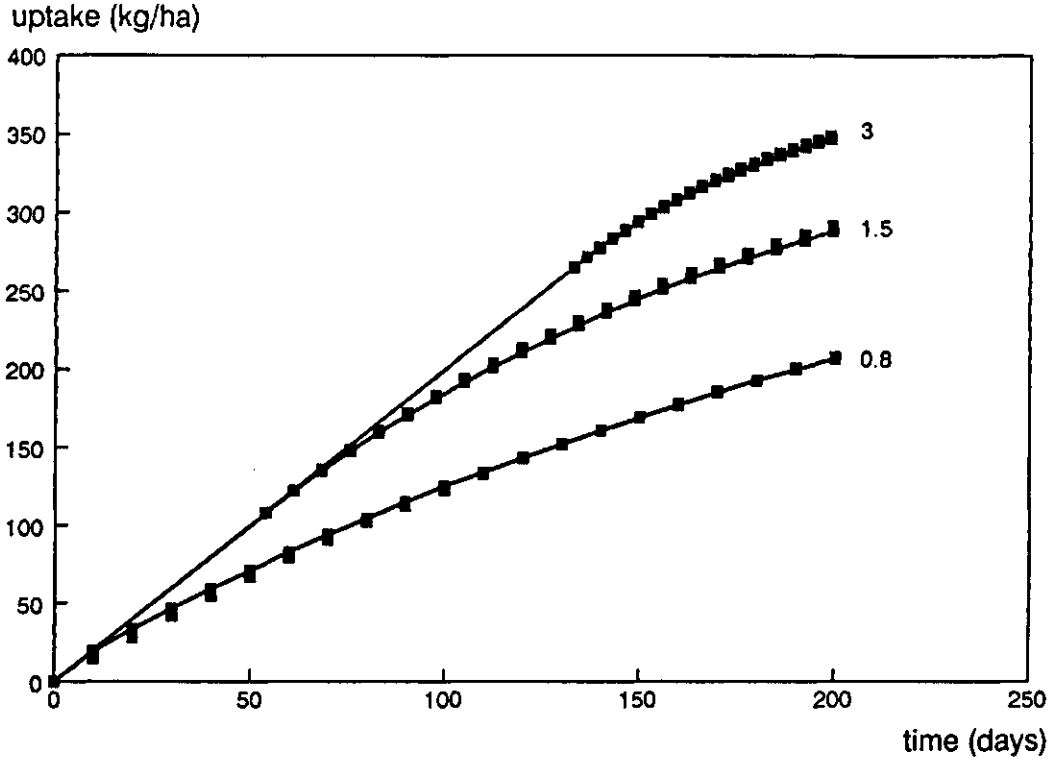


Figure 1. Cumulative uptake calculated with the exact solution (6) and the steady-rate approximation. Parameters: available amount 400 kg/ha, required uptake rate 2 kg/(ha.day), root length 20 cm, root radius 0.02 cm, transpiration 0.5 cm/day, diffusion coefficient 0.028 cm²/day, adsorption constant 20 ml/cm³. The lines give the exact solution; the points the steady-rate approximation. The figures at the curves denote the root length density in cm/cm³.

2.3. Water

Mathematical formulation

The partial differential equation describing transport of water in the soil (Richards equation) is strongly nonlinear, which makes the finding of analytical solutions generally very difficult. We had to resort to numerical techniques to obtain a solution (see Appendix II).

As shown earlier (De Willigen and Van Noordwijk, 1987) the numerical solution can be very well approximated by a steady-rate approximation similar to that given in (2), be it that it should be written in terms of the matric flux potential, which is defined as:

$$\Phi = \int_{\theta}^{\theta_{\text{sat}}} D_w d\theta - \int_P^0 K dP, \quad (11)$$

and that the limit for $\nu \rightarrow 0$ of (2) should be taken. The steady-rate solution in terms of the matric flux potential reads:

$$\Phi = \Phi_{rs} + \frac{\rho^2}{2\eta} ER_0 \left(\frac{r^2-1}{2(\rho^2-1)} - \frac{\rho^2 \ln r}{\rho^2-1} \right) \quad (12)$$

where Φ_{rs} is the matric flux potential at the root surface. The flow of water towards the root is then given as:

$$U_2 = \frac{H}{R_1^2} (\Phi_{rs} - \Phi) \frac{\rho^2-1}{G(\rho, 0)} \quad (13)$$

where $G(\rho, 0)$ is the function $G(\rho, \nu)$ given earlier for $\nu \rightarrow 0$.

Figure 2 shows the time course of water uptake in case of constant water uptake until P_{rs} , the pressure head at the root surface, equals 0.5 MPa, whereas thereafter P_{rs} is kept constant at 0.5 MPa, calculated with the numerical model and with the steady-rate approximation (13). The approximation is shown to be quite satisfactory.

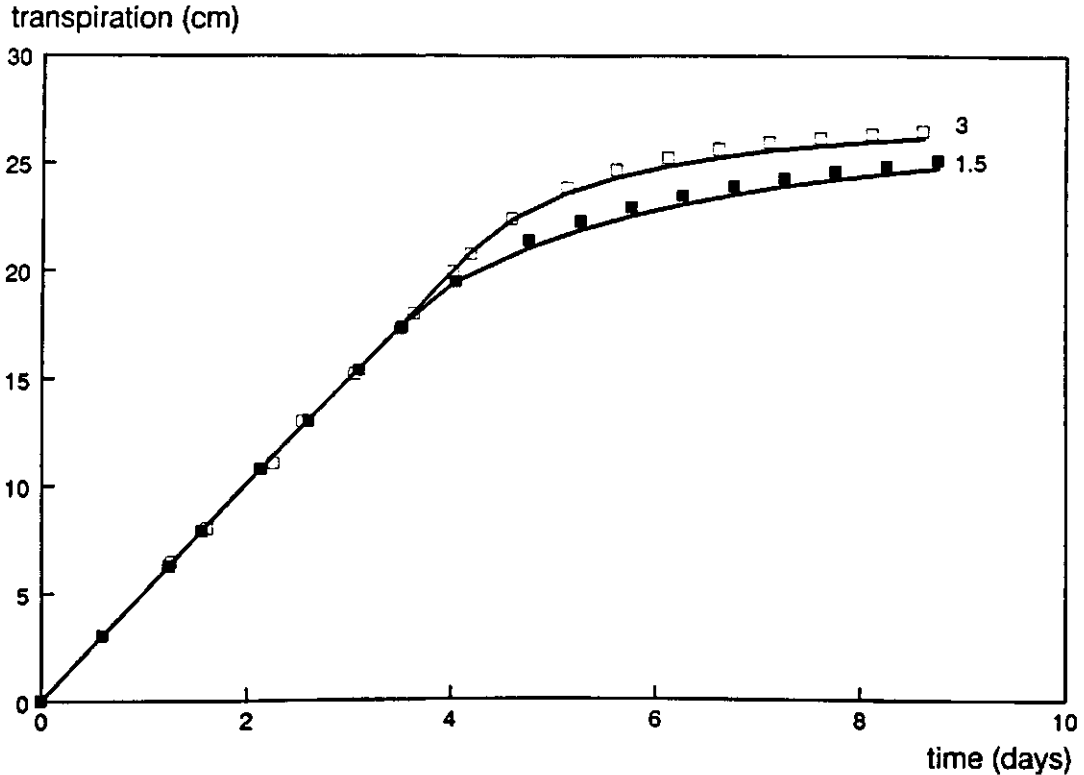


Figure 2. Cumulative transpiration calculated with the numerical model (lines) and with the steady-rate approximation (points). Transpiration was set constant at 0.5 cm/day, until the pressure head at the root surface reaches 5000 cm. Thereafter the pressure head is kept constant at 5000 cm. The figures at the curves denote the root length density in cm/cm^3 .

3. DESCRIPTION OF UPTAKE IN A MACROSCOPIC MODEL

3.1. *Nutrients*

The findings discussed in 2.2 can be used to describe uptake in a macroscopic model, i.e. a model which deals with average values of concentration and root density in horizontal layers. We first consider a single layer with uniformly distributed roots. The potential uptake rate from this layer is given by (7), i.e. the uptake rate in the zero-sink situation. As long as this potential uptake rate exceeds the required uptake rate the actual uptake rate equals the required uptake rate. When the potential uptake rate is lower than the required uptake rate, actual uptake rate equals potential uptake rate. The actual uptake rate is thus the minimum of the required and the potential uptake rate. The total uptake then simply is the sum of the uptake of the individual roots.

When different horizontal layers in the root zone are distinguished, each with its own root density and nutrient concentration the situation is more complicated. It is conceivable, as indeed is often found, that roots in favourable position can compensate for roots in less favourable position (De Jager, 1985). It is assumed therefore that the uptake rate of roots in a certain layer depends on the uptake potential of roots in other layers.

Uptake now is calculated in an iterative way. First (step 1) the nutrient demand is divided by the total root length to obtain the required uptake per unit root length. Multiplying this by the root length in a given layer yields the required uptake from that layer. If the potential uptake rate exceeds the required uptake rate, uptake from this layer equals the required uptake. If the potential uptake rate is less than the required uptake rate, uptake from this layer equals the potential uptake rate. For convenience, those layers where actual uptake equals potential uptake will be indicated as layers of category 1.

The total uptake by the root system is the sum of the uptake rates of the individual layers. If the uptake in each layer can proceed at the required rate, total uptake equals nitrogen demand and no iteration is required. If total uptake is less than nitrogen demand, it is checked whether uptake from those layers where the concentration was sufficiently high to meet the original demand (for that particular layer) can be raised to increase total uptake, possibly enough to meet the total demand.

This is achieved as follows. In step 2, first the difference between demand and total uptake, as calculated in step 1, is divided by the total root length of those layers (category 2) that were able to satisfy the required uptake rate of step 1. This yields an additional uptake rate. The

required uptake rate for layers of category 2, in step 2, now equals the required uptake rate of step 1, augmented with the additional uptake rate. It now is examined if the layer can satisfy the required uptake, i.e. if its potential uptake rate still exceeds the new value of the required uptake rate. If not, uptake rate from this layer equals potential uptake rate. If all layers of category 2 can satisfy the required uptake of step 2, total uptake equals demand and the iteration ends. If none of the layers of category 2 can satisfy the required uptake of step 2, i.e. if in all layers of category 1 and 2 zero-sink uptake occurs, the iteration also ends. If only a part of the layers of category 2 can satisfy the required uptake of step 2, iteration proceeds to step 3, etc. Appendix III describes the computerprogram of this procedure in detail.

This calculation procedure implies that roots growing under favourable conditions will compensate as much as possible for roots growing under less favourable conditions. It is thus assumed that information about the necessary behavior, as far as uptake is concerned, is instantaneously available throughout the complete root system.

The procedure described above can also be applied when roots within a horizontal layer are not distributed uniformly. The layer then is divided over a number of compartments within which root distribution can be assumed uniform.

3.2 Water

As in 3.1 we start with considering a single layer of soil containing vertical and uniformly distributed roots. The flow of water over the root surface is supposed to be linearly related to the difference between the plant water potential and the pressure head of the soil water at the root surface (De Willigen and Van Noordwijk, 1987):

$$F_w = k_1 (P_{rs} - P_p) + k_2 \quad (14)$$

where F_w is the flux of water in $\text{cm}^3/(\text{cm root.day})$, P_{rs} is the pressure head in the soil at the root surface in cm, P_p is the plant water potential in cm, and k_1 in cm/day and k_2 in $\text{cm}^3/(\text{cm root.day})$ are coefficients related to the root conductivity.

If the thickness of the soil layer is Δx cm and the root length density L_{rv} cm/cm^3 , the uptake U_1 in cm^3 water per cm^2 soil surface per day is given by:

$$U_1 = L_{rv} \Delta x F_w = q(P_{rs} - P_p) + v \quad (15)$$

where

$$q = L_{rv} \Delta x k_1, \text{ and } v = L_{rv} \Delta x k_2$$

We assume that no water can accumulate at the root surface, so that U_1 equals the supply of water at the root surface. The flow from the bulk soil in the layer with matric flux potential Φ towards the root surface where the matric flux potential is Φ_{rs} is given by (cf (13)):

$$U_2 = s(\Phi_{rs} - \Phi) \quad (16)$$

where

$$s = \frac{\Delta x}{R_1^2} \frac{(\rho^2 - 1)}{G(\rho, 0)}$$

whereas there exists a functional relationship between Φ and P (see definition of Φ in (11)).

If the required uptake is given as E_{act} (the transpiration rate in cm/day) the right hand side of (16) should equal E_{act} , and the resulting equation can simply be solved for Φ_{rs} . Using the inverse of (11) then P_{rs} is calculated. Finally because:

$$U_1 = U_2 = E_{act}$$

the plant water potential can be computed from (15) as:

$$P_p = P_{rs} - (E_{act} - v)/q \quad (17)$$

The situation is in fact more complicated because the actual transpiration rate is a function of the plant water potential:

$$E_{act} = f(P_p) E_{pot} \quad (18)$$

where $f(P_p)$ is a factor by which the potential transpiration E_{pot} has to be reduced. As $f(P_p)$ is a non-linear function of P_p , E_{act} and P_{rs} have to be found by iteration.

When the root system is distributed over n different layers, but roots can be assumed to be distributed uniformly within a layer, for each layer equations like (15) and (16) can be formulated. Equating these equations one finds for the i -th layer:

$$q_i(P_{rs,i} - P_p) + v_i = s_i(\Phi_{rs,i} - \Phi_i) \quad (19)$$

It is assumed that the plant water potential P_p is identical everywhere in the root system. In total then one obtains n equations of the form of (19), and $n+1$ unknowns i.e. $P_{rs,1} - P_{rs,n}$ (where again (11) can be used to calculate Φ from P or vice-versa) and P_p . When the uptake rate E_{act} is known an additional equation states that the sum of the flows over the rootsurface in each layer from the root zone equals E_{act} :

$$\sum_{i=1}^n q_i(P_{rs,i} - P_p) + v_i = E_{act} \quad (20)$$

When one takes into account the relation between plant water potential and uptake rate equation (18) has to be used. Because of the non-linearity of (11) and (18) the solution has to be found by iteration. Appendix IV gives the details.

4. PROGRAMS

Calculations were performed with the computerprograms shown in appendices I-IV. All programs are written in Fortran. The programs consist of a number of subprograms (Fortran subroutines and functions), each dealing with a specific part of the calculations. The programs are organized and documented according to recommendations of Van Kraalingen and Rappoldt (1989).

5. EXAMPLES

5.1 Water uptake

As an example results of Sharp and Davies (1985) will be used. They performed an experiment on water uptake and root growth of maize plants. Individual plants were grown in soil columns of 80 cm height. After a preliminary growth period of two weeks the plants were subjected to two treatments. Half of the plants were watered daily, where care was taken that the soil water was replenished up to field capacity, the other half did not get any water at all for the 18 day experimental period. Every three days some columns were harvested and soil water content, root length distribution, total dry matter and its distribution were measured, as well as, prior to harvesting, the leaf water potential. Soil water depletion rates were calculated from the changes in soil water content between successive sampling days.

No data on diffusivity as a function of water content are given, and the information about the moisture retention curve is rather incomplete. Nevertheless, the data can be used to illustrate the performance of the model. To this end the model was run with data on hydraulic properties of

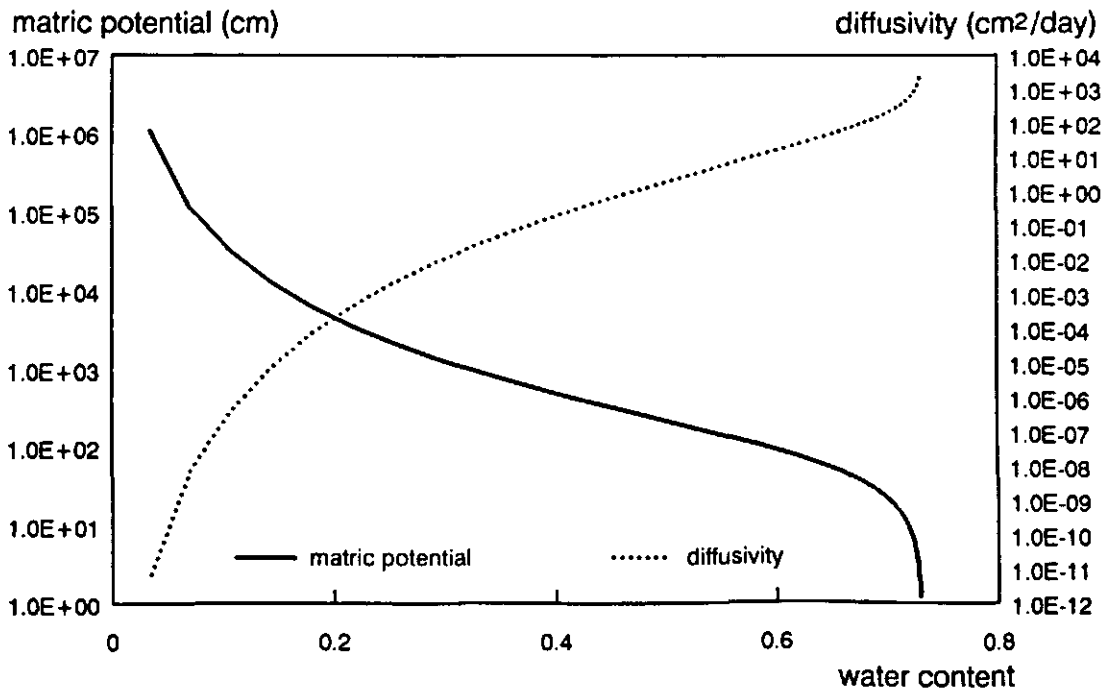


Figure 3. Relation between matric potential, diffusivity and water content for a peat soil (no B16 in the Staring Series (Wösten, 1987)).

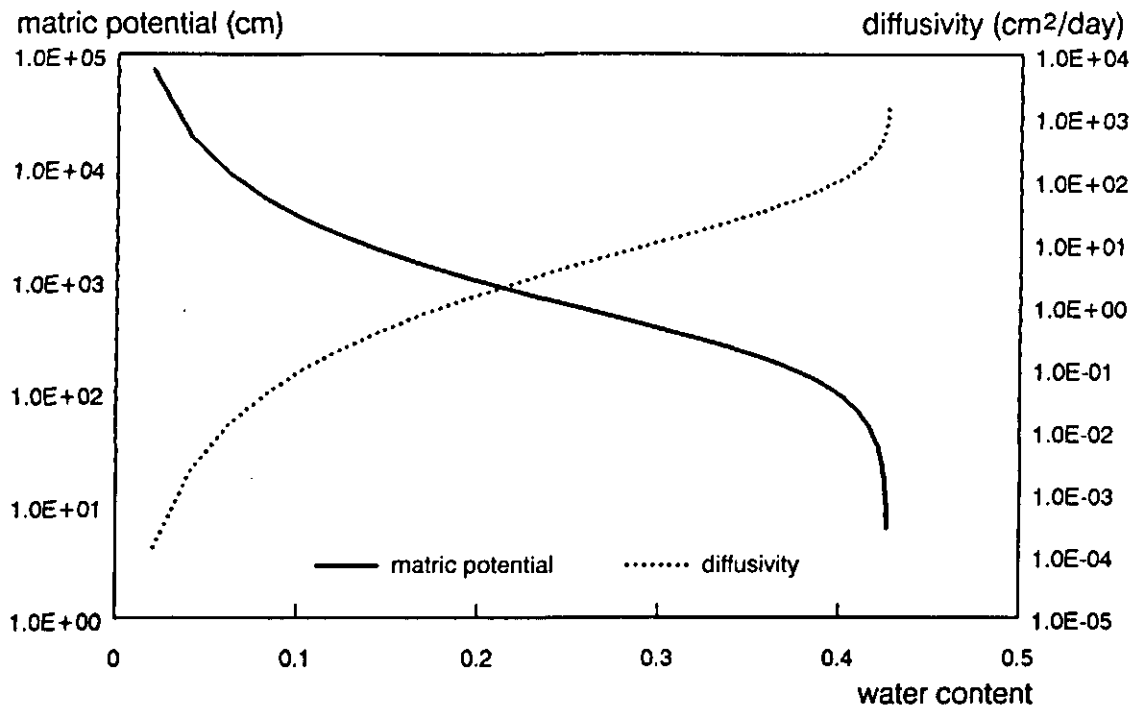


Figure 4. Relation between matric potential, diffusivity and water content for a sandy loam (Lov12c data from Boekhold, 1987).

two soils: one a sandy loam (Lov12c; Boekhold, 1987) the other a peaty soil (Bl6; Wösten, 1987). Figures 3 and 4 depict the relation between water content, pressure head and diffusivity of these two soils.

Figures 5 and 6 give the results for day 15 for the two treatments. In the treatment where the soil was kept at field capacity (figure 5) distribution of uptake with depth was similar to the root density distribution. In the calculations it was assumed that soil water was in equilibrium with a groundwater table at a depth of 80 cm, the length of the soil tube. According to the calculations at every depth in the transport chain: bulk soil \rightarrow root surface \rightarrow root, the highest resistance was experienced by the transport over the root wall. The overall resistance was therefore lowest where root density was highest, which results in uptake being more or less proportional to root density. Because of the dominance of the root resistance the results for the two soils were practical identical, differences in calculated uptake being less than 0.01%.

The results for the unwatered treatment are given in figure 6. The pressure head at every depth was estimated from the reported water content. Now the soil resistance is, except for the deepest layer, higher than the root resistance, so distribution of uptake is quite different from root density distribution. Moreover, the results for the two soils now clearly

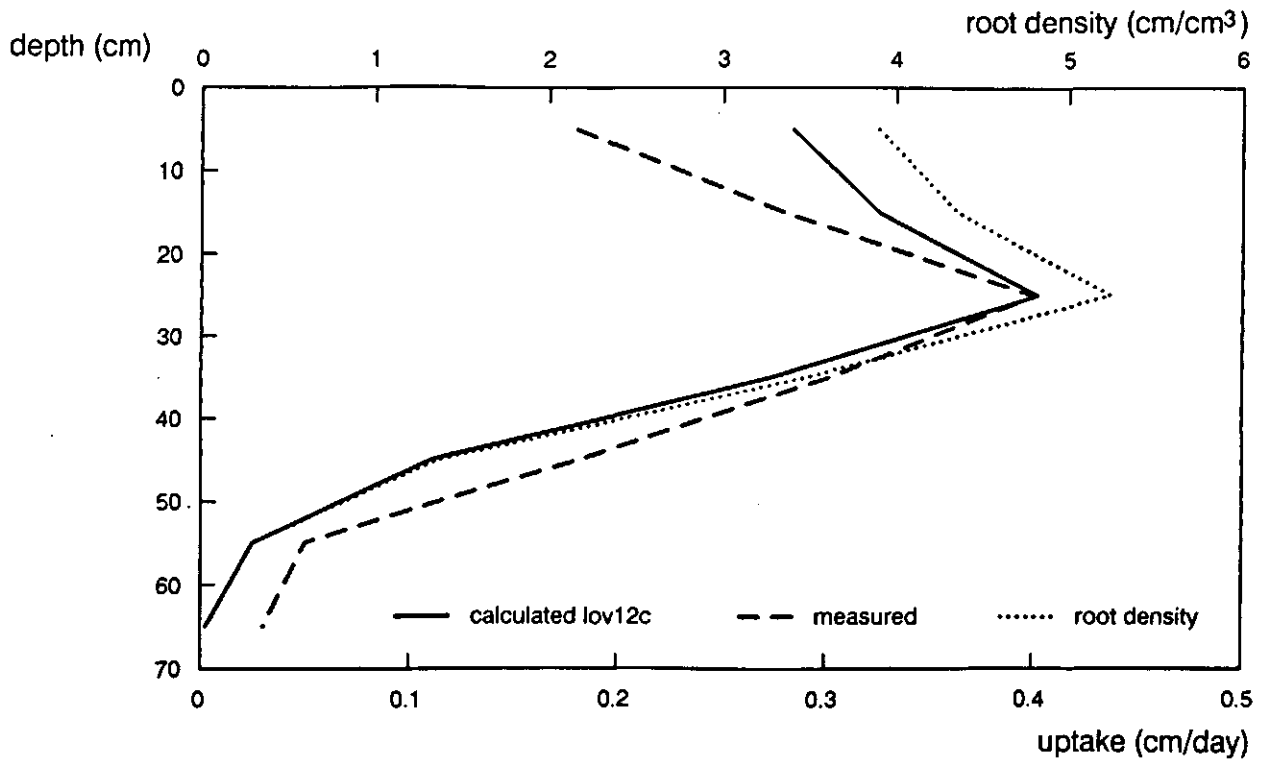


Figure 5. Measured and calculated depth-distribution of water uptake and root-density of a maize-plant in a soil kept at field capacity. Data from Sharp and Davies (1985). For the calculations the hydraulic properties of Lov12c (figure 4) have been used.

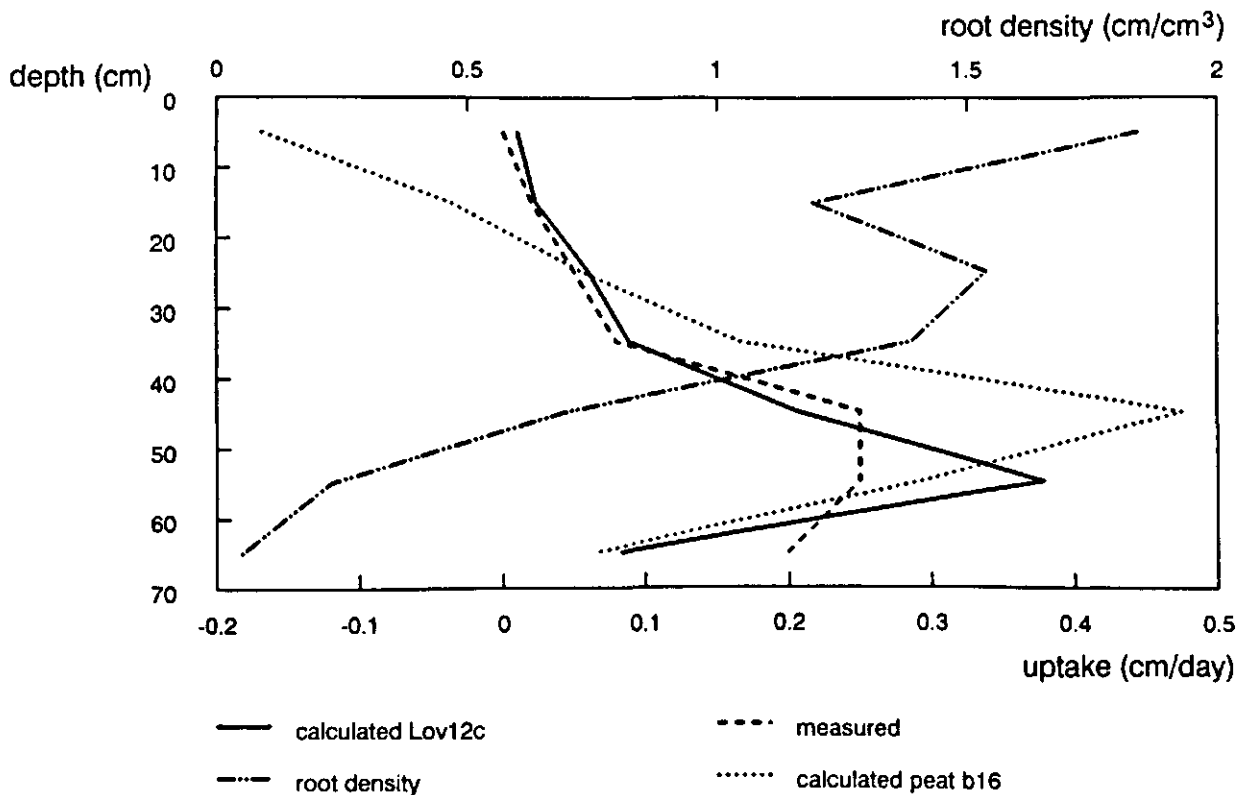


Figure 6. As figure 5, but in a soil which has not been watered during 15 days. For the calculations the hydraulic properties of Lov12c (figure 4) and B16 (figure 3) have been used.

differ, those for Lov12c being more or less similar to the measured results. The results of the peat B16 differ considerably from the measurements. On this soil in the upper two layers negative water uptake occurs according to the calculations, i.e. water flows out of the root to the soil. This may be an artefact due to the assumption of uniform plant water potential, but on the other hand such a phenomenon is often established experimentally (e.g. Baker and Van Bavel, 1986).

5.2. Nutrient uptake

To illustrate the possibilities of the nutrient uptake model, the water uptake pattern and water content distribution as found by Sharp and Davies (1985) discussed in 5.1 were used.

Four situations were considered: the two treatments of water application mentioned in section 5.1 with the corresponding root length distributions, and two different distributions of mineral nitrogen in the soil. In one of the chosen distributions every soil layer contains 1 kg/ha, except the upper 10 cm where mineral nitrogen amounts to 20 kg/ha, in the other this amount is found in the layer 40-50 cm. The required uptake rate of the maize plants was estimated from the transpiration rate assuming a transpiration coefficient of 350 kg/kg and an assumed nitrogen content of 2.5%. For the adequately watered plants the required uptake calculated in this fashion amounted to 8.8 kg/(ha.day), for the unwatered plants to 6 kg/(ha.day).

The effective diffusion coefficient of ions in soil is strongly influenced by the water content. It can be calculated as:

$$D = D_0 f_1 \theta \quad (21)$$

where D_0 is the diffusion coefficient of the ion in free water, and f_1 an impedance factor. The latter is a function of θ as well. Figure 7 gives the diffusion coefficient as a function of the water content using the relation between impedance factor and water content as established by Barraclough and Tinker (1981) for sandy and sandy loam soils. This relation has been used in the model calculations.

Figures 8 and 9 show the results. For the adequately watered plants the distribution of nitrogen has no effect, whereas in the dry situation concentration of nitrogen in deeper moister layers is much more favourable, the realized uptake rates being 1.5 and 4.5 kg/(ha.day) respectively.

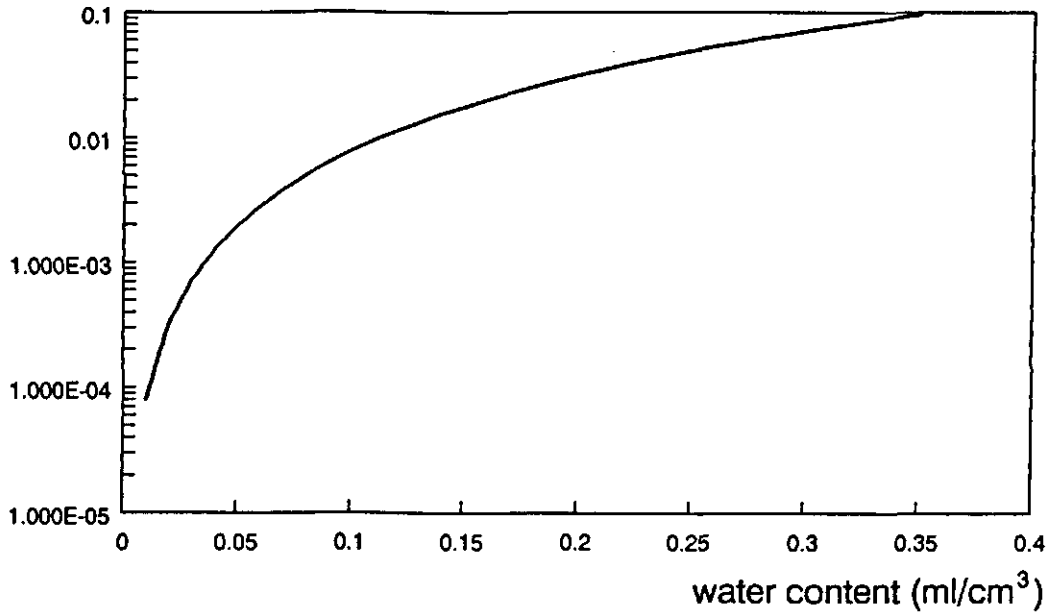
diffusion coeff. (cm^2/day)

Figure 7. Diffusion coefficient of a nutrient, the diffusion constant of which in water is $0.5 \text{ cm}^2/\text{day}$, as a function of water content for sandy soils. After Barraclough and Tinker (1981).

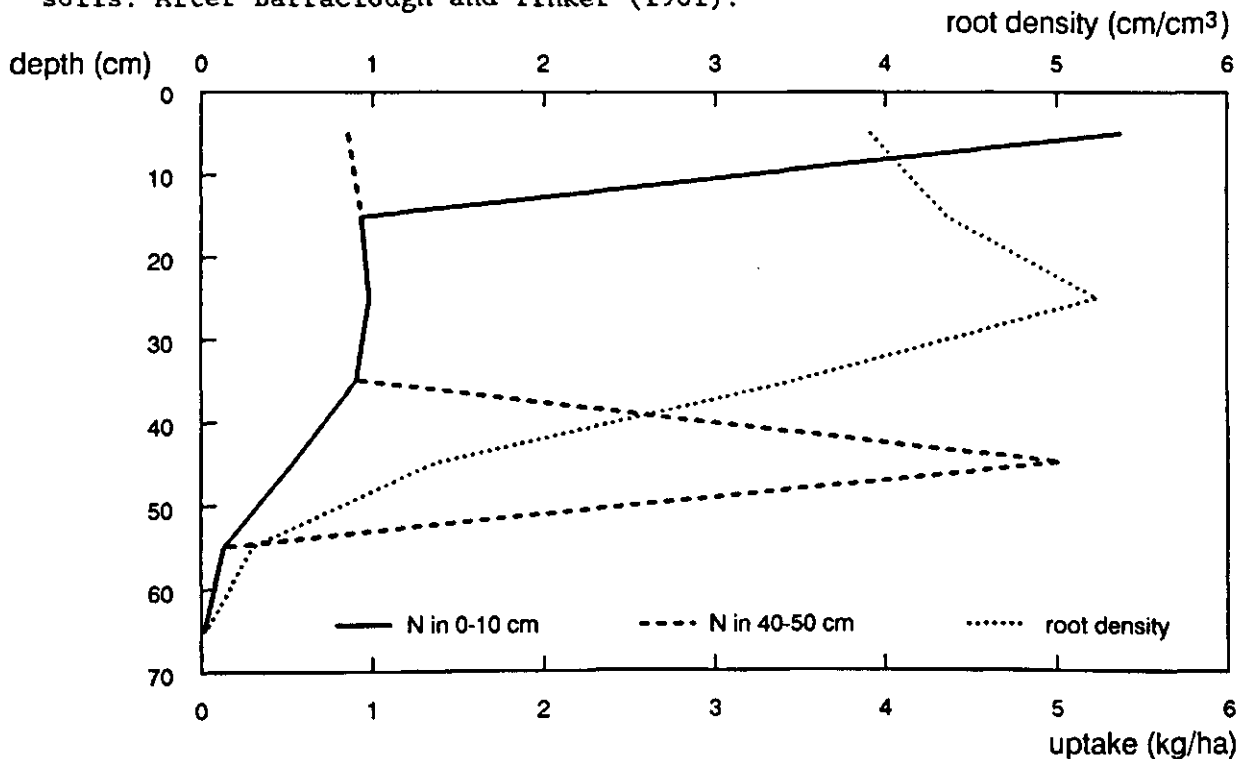


Figure 8. Distribution of nitrate-N uptake and root length density with depth as calculated with the model UPTA in a soil at field capacity. Water-uptake distribution as in figure 5 (measurements). Diffusion coefficient calculated from watercontent as shown in figure 7. All soil layers contain 1 kg of nitrate-N per ha, except for the layer 0-10 cm (continuous line) or 40-50 cm (interrupted line). These layers contain 20 kg nitrate-N per ha. Nitrogen demand: $8.8 \text{ kg}/(\text{ha} \cdot \text{day})$.

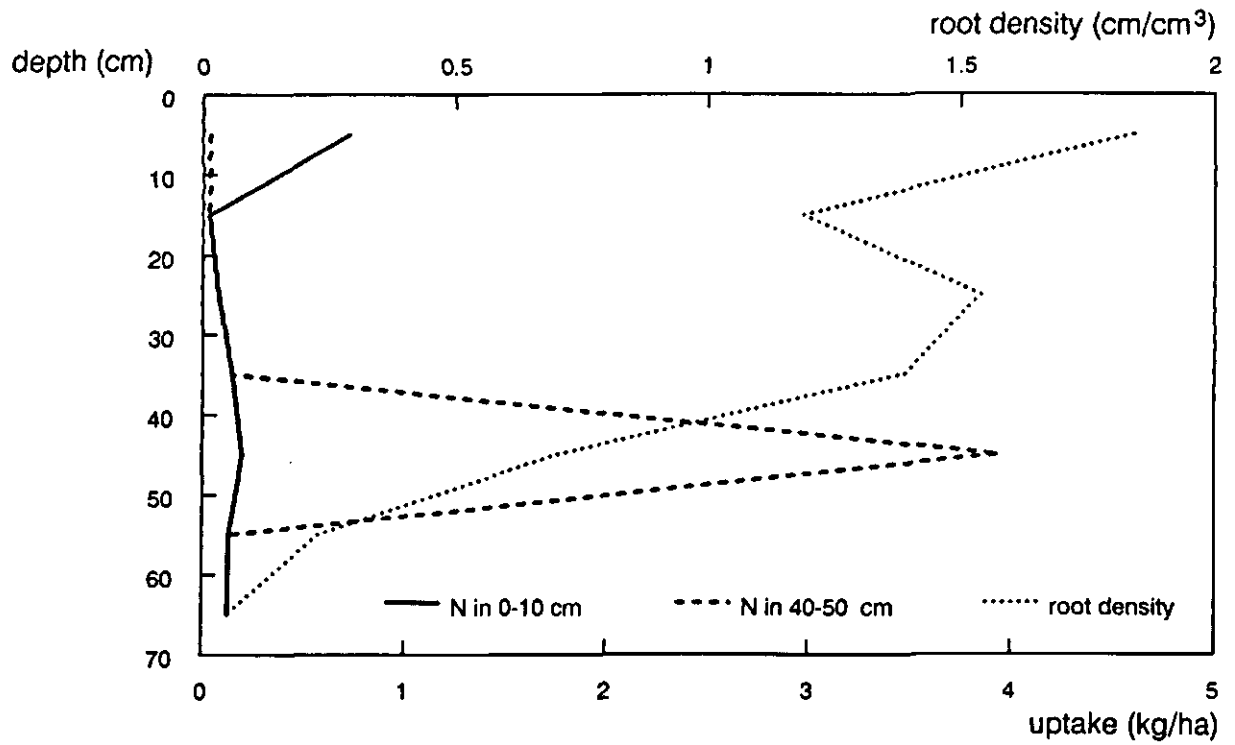


Figure 9. As fig 8 but in a soil which has not been watered during 15 days. Water-uptake distribution as in figure 6 (measurements). Nitrogen demand: 6 kg/(ha.day).

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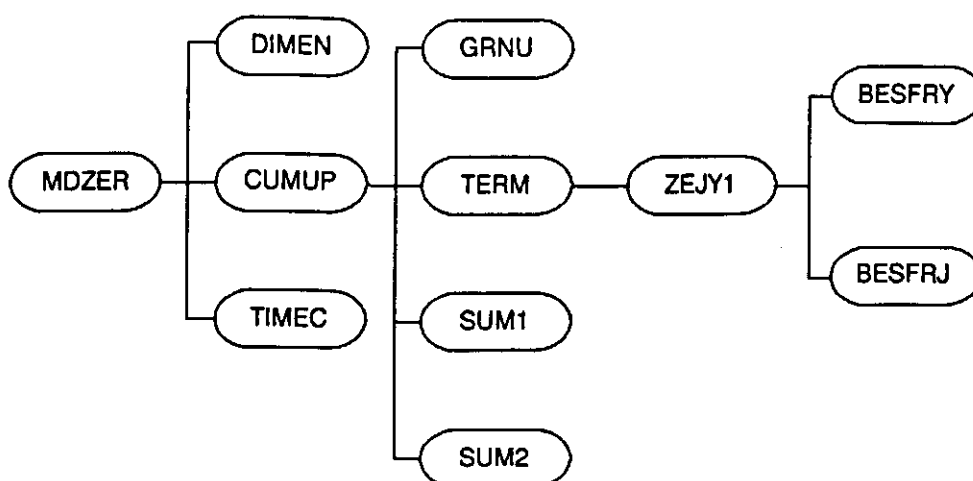
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APPENDIX I. Calculation of the nutrient uptake by a single root in a zero-sink situation.

The relation between the subroutines is given in figure AI-1.

The subroutine DIMEN calculates dimensionless parameters ρ , η , ϕ . These are used in TIMEC, which calculates the period of unconstrained uptake both in dimensionless and absolute units.

Relational diagram of subroutines in MDZER



The core of the program is formed by the subroutine CUMUP which calculates the uptake and cumulative uptake after the period of unconstrained uptake, both exact and approximately. When the period of unconstrained uptake is less than zero, indicating that the concentration at the root surface drops to zero before a steady-rate situation has been developed, the calculations pertain to (9) and (10), otherwise to (4) and (5). CUMUP calls TERM, which calculates the terms of the summation series of (4), (5), (9), and (10), thereby using subroutine ZEJY1 which calculates the zero's α_n of the crossproduct given in the context of (3).

In the program the uptake rate (UP), the cumulative uptake (TUP), and their approximations (UPAP resp. TUPAP) are calculated in non-dimensionless form. In case of zero-sink uptake from the beginning the uptake rate in kg/(ha.day) is calculated as:

$$UP = 100 \frac{2HDC_i}{R_1^2} \omega_t$$

and a similar expression is used to calculate TUP. The factor 100 converts the units from mg/cm² to kg/ha.

If the period of unconstrained uptake is larger than zero, UP is calculated using:

$$UP/UPR = w_t/w$$

where UPR is the uptake rate (in kg/ha) in the period of unconstrained uptake. The cumulative uptake TUP is the sum of the total uptake in the period of unconstrained uptake and the integral of UP in time.

```

*-----*
* Program MDZER.FOR *
* Purpose: Calculation of diffusion and massflow of a nutrient *
* to a root. Zero-sink solution. Replenishment of water at outer boundary *
* FORMAL PARAMETERS: (I=input,O=output,C-control,IN-init,T-time) *
* name type meaning units class *
*-----*
* R0 R4 radius root cm I *
* D0 R4 diffusion coefficient in free water cm2/day I *
* DIF R4 diffusion coefficient in soil cm2/day 0 *
* CF1 R4 coefficients for relation between *
* CF2 R4 impedance and water content *
* TFAC R4 ratio between real and dimensionless time day 0 *
*
* SUBROUTINES called: *
* DIMEN: calculates dimensionless variables *
* TIMEC: calculates time constants *
* CUMUP: calculates uptake rates *
*
* File usage: *
* MDZER.INP: contains input-data *
* MDZER.OUT: detailed output on uptake, cumulative uptake, parameters *
*-----*

```

```

REAL LRV(20),TIME(50),UP(50)
REAL UPAP(50),TUP(50),TUPAP(50)
INTEGER NC(20)
REAL NU

```

```

*-----*
* Input data
DATA TOL,D0/1.E-5,0.5/

OPEN (FILE='MDZER.OUT',UNIT=45)
OPEN (FILE='MDZER.INP',UNIT=40)
OPEN (FILE='MASZER.LOG',UNIT=46)

CALL MOFILP(40)
READ (40,*) NLRV
CALL MOFILP(40)
READ (40,*) (LRV(I),I=1,NLRV)
CALL MOFILP(40)
READ (40,*) R0
CALL MOFILP(40)
READ(40,*) HSC
CALL MOFILP(40)
READ (40,*) AK
CALL MOFILP(40)
READ (40,*) TRANSP
CALL MOFILP(40)
READ (40,*) PAVAM

```

```

      CALL MOFILP(40)
      READ (40,*) UPR
      CALL MOFILP(40)
      READ (40,*) WC
      CALL MOFILP(40)
      READ(40,*) CF1,CF2,WLOW
*
      PI=4.*ATAN(1.)

*----- calculation of diffusion coefficient as a function of
*----- water content, FIMP = impedance factor
      IF(WC.GE.WLOW)THEN
        FIMP=CF1*WC+CF2
      ELSE
        FIMP=(CF1*WLOW+CF2)*WLOW*WC
      ENDIF
      DIF=D0*WC*FIMP
      TFAC=R0**2/DIF

      WRITE (45,100)
      WRITE(45,101) TRANSP,PAVAM,UPR,AK,WC,DIF

10    CONTINUE

*----- DO 25 over root densities
      DO 25 IL=1,NLRV
        CALL DIMEN(IL,LRV,R0,TRANSP,HSC,DIF,PAVAM,AK,WC,UPR,
1          R1,RHO,NU,CII,CT,AAA,BUF,PHI,ETA,COF)
        TNU=2.*NU

        CALL TIMEC(RHO,ETA,PHI,BUF,TNU,TFAC,TAUM,TAUD,TAUNU,FDD,FDNU,
1          CUD,CUNU)

        CALL CUMUP(20,RHO,TFAC,TAUM,TAUNU,UPR,BUF,TNU,
1          COF,R1,HSC,CII,DIF,TIME,UP,UPAP,TUP,TUPAP)

        WRITE(45,102) (TIME(I),UP(I),UPAP(I),TUP(I),
          $          TUPAP(I),I=1,21)

25    CONTINUE

100   FORMAT(/1X,'PARAMETERVALUES:')
101   FORMAT(1X,'TRANSP  ='F7.2,1X,'CM/DAY'/
1     1X,'PAVAM   ='F7.1,1X,'KG/HA'/
2     1X,'UPR    ='F7.1,1X,'KG/(HA.DAY)'/
3     1X,'AK     ='F7.1/1X,'WATERCONTENT  ='F8.2/
4     1X,'DIF. COEFF ='1PE15.5)

102   FORMAT(
1     /12X,'TIME',13X,'UP',11X,'UPAP',12X,'TUP',10X,'TUPAP'
2     /(1X,1P5E15.5))
      STOP
      END

```

```

*-----*
* Subroutine TIMEC                                     *
* Purpose: Calculation time constants, period of unconstrained uptake, *
*          maximum uptake period and related parameters                *
*-----*
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time)      *
* name   type meaning                                           units  class *
*-----*-----*-----*-----*-----*
* RHO    R4    Dimensionless radius soil cylinder              -      I    *
* ETA    R4    Dimensionless root length                        -      I    *
* PHI    R4    Dimensionless supply parameter                  -      I    *
* NU     R4    Dimensionless flux of water                      -      I    *
* BUF    R4    Buffer capacity                                   -      I    *
* TAUM   R4    Dimensionless maximum period of unconstrained      -      0    *
*          uptake                                                *
* TAUD   R4    Dimensionless period of unconstrained uptake      -      0    *
*          transport by diffusion only                            *
* TAUNU  R4    Dimensionless period of unconstrained uptake      -      0    *
*          transport by diffusion and massflow                    *
* FDD    R4    Fractional depletion by unconstrained uptake      -      0    *
*          transport by diffusion only                            *
* FDNU   R4    Fractional depletion by unconstrained uptake      -      0    *
*          transport by diffusion and massflow                    *
* CUD    R4    Fraction left at end of period of unconstrained  -      0    *
*          uptake, transport by diffusion only                    *
* CUNU   R4    Fraction left at end of period of unconstrained  -      0    *
*          uptake, transport by diffusion and massflow            *
*-----*
* Subroutines called : none                                         *
* Functions called :                                              *
*   GRNU: calculates G-function                                     *
*-----*
* File usage: time constants written to MDZER.OUT                  *
*-----*

```

```

SUBROUTINE TIMEC(RHO,ETA,PHI,BUF,TNU,TFAC,TAUM,TAUD,TAUNU,FDD,
1              FDNU,CUD,CUNU)

```

```

*-----*
*-----* Calculation period of unconstrained
*-----* uptake TAUNU, maximum TAUM
*
RHO2=RHO**2
TAUM=(RHO2-1.)/RHO2*ETA*PHI
TAUD=TAUM-BUF*GRNU(0.,RHO)
TAUNU=TAUM-BUF*GRNU(TNU,RHO)
FDNU=TAUNU/TAUM
FDD=TAUD/TAUM
CUNU=1.-FDNU
CUD=1.-FDD
*
TM=TFAC*TAUM

```

```
TD=TFAC*TAUD
TN=TFAC*TAUNU
WRITE(45,206) TM,TAUM,TD,TAUD,TN,TAUNU
206  FORMAT(/15X,'TIME-CONSTANTS'/31X,'DAYS',11X,'DIML'
1      /1X,'MAXIMUM:'12X,1P2E15.5/1X,'DIFFUSION : '9X,1P2E15.5
2      /1X,'DIF. AND MASS FLOW : '1P2E15.5)

RETURN
END
```

```

*-----*
* Subroutine DIMEN
* Purpose: calculation of dimensionless parameters
* FORMAL PARAMETERS: (I=input,O=output,C-control,IN=init,T=time)
* name      type meaning                      units  class
*-----*
* LRV       R4   Root length density          cm/cm3   I
* RO        R4   Radius root                  cm       I
* TRANSP    R4   transpiration rate           cm/day   I
* HSC       R4   Root length                  cm       I
* DIF       R4   Diffusion coefficient soil    cm2/day  I
* PAVAM     R4   Potential available amount of nutrient kg/ha    I
* AK        R4   Adsorption constant nutrient -       I
* WC        R4   Water content                -       I
* UPR       R4   Uptake rate nutrient          kg/(ha.day) I
* R1        R4   Radius soil cylinder          cm       0
* RHO       R4   Dimensionless radius soil cylinder -       0
* NU        R4   Dimensionless flux of water   -       0
* CII       R4   Initial concentration nutrient mg/ml    0
* CT        R4   Bulk density of nutrient     mg/cm3    0
* AAA       R4   Uptake rate                   mg/(cm2.day) 0
* BUF       R4   Buffer capacity                -       0
* PHI       R4   Dimensionless supply parameter -       0
* ETA       R4   Dimensionless root length     -       0
*
* Subroutines/Functions called:none
*
* File usage: dimensionless parameters written to MDZER.OUT
*-----*

```

```

SUBROUTINE DIMEN(IL,LRV,RO,TRANSP,HSC,DIF,PAVAM,AK,WC,UPR,
1 R1,RHO,NU,CII,CT,AAA,BUF,PHI,ETA,COF)
  DIMENSION LRV(30)
  REAL LRV,NU

  PI=4.*ATAN(1.)
  R1=1./SQRT(PI*LRV(IL))
  RHO=R1/RO
  RHO2=RHO**2
  TNU=R1**2*TRANSP/(2.*DIF*HSC*(RHO2-1.))*(RHO2-1.)
  NU=TNU/2.
  BUF=WC+AK
  CII=0.01*PAVAM/(HSC*BUF)
  CT=CII*BUF
  AAA=UPR/100.
  PHI=DIF*CT/(AAA*RO)
  ETA=HSC/RO
  COF=4.*(NU+1.)/(RHO**2*(TNU+2.))-1.)

  WRITE(45,102) LRV(IL)
  WRITE(45,103) R1,RHO,RHO2,PHI,ETA,TNU
  RETURN

```

```
102  FORMAT(//'***** LRV = '1PE15.5,2X,'*****'/
      1      1X,'COMBINED AND DIMENSIONLESS PARAMETERS')
103  FORMAT(1X,'R1      ='1PE15.5,1X,'CM'/1X,'RHO  ='1PE15.5,
      1      1X,'RHO2  ='1PE15.5/1X
      2      'PHI   ='1PE15.5/1X,'ETA  ='1PE15.5,1X/1X
      3      'TNU   ='1PE15.5)

      END
```



```

*-----*
* Subroutine TERM *
* Purpose: calculates N terms form the series part of zero-sink solution *
*           concerning uptake of nutrients. The terms TE1 and TE2 pertain *
*           to steady-rate initial condition, TE3 and TE4 to constant *
*           initial condition *
* FORMAL PARAMETERS: (I=input,O=output,C-control,IN=init,T=time) *
* name  type meaning                                units  class *
*-----*-----*-----*-----*-----*
* RHO    R4  dimensionless root density, i.e. the radius      -      I  *
*           of the soil cylinder R1 over the root radius      *
*           R0 *
* FL     R4  Dimensionless flux of water                      -      I  *
* TE1    R4  Term of solution for integrated uptake           -      0  *
* TE2    R4  Term of solution for uptake rate                 -      0  *
* TE3    R4  Term of solution for integrated uptake           -      0  *
* TE4    R4  Term of solution for uptake rate                 -      0  *
* N      I4  Number of terms                                  -      I  *
* AL     R4  Zero's from crossproduct of Bessel-functions:    -      0  *
*            $Y(FL,AL)J(FL+1,AL) - J(FL,AL)Y(FL+1,AL) = 0$  *
* * *
* Subroutines called: *
* ZEJY1 : calculates zero's from crossproduct of Bessel-functions: *
*            $Y(FL,AL)J(FL+1,AL) - J(FL,AL)Y(FL+1,AL) = 0$  *
* BESFRJ : Bessel function of first kind and fractional order *
* * *
* Functions called: none *
* * *
* File usage: none *
*-----*

SUBROUTINE TERM(RHO,FL,TE1,TE2,TE3,TE4,N,AL)
REAL TE1(N),TE2(N),TE3(N),TE4(N),AL(N),BJ(2)
REAL JNA,JN1RA

DO 5 I=1,N
*-----* Calculation of AL(I)
CALL ZEJY1(AL(I),I,RHO,FL,20.,1.E-5,6)
WRITE(46,*) 'I, AL ',I,AL(I)
*-----*
*-----* Calculation of Bessel function J, with order FL
*-----* and argument AL(I)
CALL BESFRJ(AL(I),FL,6,BJ)
JNA=BJ(1)

*-----* Calculation of Bessel function J, with order FL+1
*-----* and argument AL(I)*RHO
RA=RHO*AL(I)
CALL BESFRJ(RA,FL,6,BJ)
JN1RA=BJ(2)

TE1(I)=JN1RA**2/(AL(I)**4*(JNA**2-JN1RA**2))
TE2(I)=TE1(I)*AL(I)**2

```

```
      TE3(I)=(2*FL*JNA*JN1RA-AL(I)*RHO**(FL+1)*JN1RA**2)/  
1      (AL(I)**3*RHO**(FL+1)*(JNA**2-JN1RA**2))  
      TE4(I)-TE3(I)*AL(I)**2  
5  CONTINUE  
  RETURN  
  END
```

```

*-----*
* Function SUM1                                           *
* Purpose: Calculates summation series of solution of integrated *
*          uptake rate, steady-rate initial condition      *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time) *
* name      type meaning                                units  class *
*-----*-----*-----*-----*
* T         R4    Dimensionless time                    -      I   *
* AL        R4    Zero's from crossproduct of Bessel-functions: -      I   *
* BUF       R4    Dimensionless buffer-capacity          -      I   *
* TE1       R4    Terms from summation series            -      I   *
* N         R4    Number of terms                        -      I   *
*-----*-----*-----*-----*
* Subroutines called: none                                *
* Functions called: none                                  *
* File usage: none                                        *
*-----*

```

```

      FUNCTION SUM1(T,TE1,AL,BUF,N)
      REAL TE1(N),AL(N)

      SUM1=0.
      DO 5 I=1,N
        TERM=TE1(I)*(1.-EXP(-AL(I)**2*T/BUF))
        SUM1=SUM1+TERM
        IF(ABS(TERM/SUM1).LT.1.E-5)GO TO 6
5      CONTINUE

6      RETURN
      END

```

```

*-----*
* Function SUM2                                         *
* Purpose: Calculates summation series of solution of uptake rate, steady- *
*           rate initial condition                     *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN-init,T=time)          *
* name      type meaning                               units  class *
* -----*
* T         R4    Dimensionless time                   -      I   *
* AL        R4    Zero's from crossproduct of Bessel-functions: -      I   *
* BUF       R4    Dimensionless buffer-capacity        -      I   *
* TE2       R4    Terms from summation series          -      I   *
* N         R4    Number of terms                      -      I   *
*-----*
* Subroutines called: none                             *
* Functions called: none                               *
* File usage: none                                     *
*-----*

```

```

FUNCTION SUM2(T,TE2,AL,BUF,N)
REAL TE2(N),AL(N)

```

```

SUM2=0.
DO 5 I=1,N
    TERM=TE2(I)*EXP(-AL(I)**2*T/BUF)
    SUM2=SUM2+TERM
    IF(ABS(TERM/SUM2).LT.1.E-5)GO TO 6
5  CONTINUE

6  RETURN
END

```

```

*-----*
* Subroutine CUMUP                                     *
* Purpose: calculates uptake rate and cumulative uptake in zero-sink *
*          situation, and their steady-rate approximations as a function *
*          of time.                                     *
*
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time) *
* name   type meaning                                     units   class *
*-----*-----*-----*-----*-----*
* NI      I4   Number of time-steps                        -        I   *
* TFAC    R4   Ratio between real and dimensionless time   day       I   *
* NU      R4   Dimensionless flux of water                 -        I   *
* BUF     R4   Buffer capacity                             -        I   *
* TAUM    R4   Dimensionless maximum period of unconstrained uptake -        I   *
* TAUNU   R4   Dimension less period of unconstrained uptake -        I   *
* UPR     R4   Required uptake rate nutrient               kg/(ha.day) I   *
* AL      R4   Zero's from crossproduct of Bessel-functions *
* TIME    R4   Time                                         days      0   *
* UP      R4   Uptake rate in zero-sink situation          kg/(ha.day) 0   *
* UPAP    R4   Uptake rate in zero-sink situation,         kg/(ha.day) 0   *
*          steady-rate approximation
* TUP     R4   Cumulative uptake                           kg/ha     0   *
* TUPAP   R4   Cumulative uptake steady-rate approximation kg/ha     0   *
*
* Subroutines called:
*   TERM: calculates terms of summation series
*
* Functions called:
*   SUM1,SUM2: produce values of summation series
*   GRNU : Calculates G-function
*
* File usage: none
*-----*

```

```

SUBROUTINE CUMUP(NI,RHO,TFAC,TAUM,TAUNU,UPR,BUF,TNU,
1 COF,R1,HSC,CII,DIF,TIME,UP,UPAP,TUP,TUPAP)
  DIMENSION TIME(30),UP(30),UPAP(30),TUP(30),TUPAP(30)
  DIMENSION TE1(50),TE2(50),TE3(50),TE4(50),AL(50)
  REAL NU

  NU=TNU/2
  CALL TERM(RHO,NU,TE1,TE2,TE3,TE4,50,AL)
  WRITE(46,*) 'TERM ',(TE4(I),I=1,20)

  TAU=TAUNU
  IF(TAUNU.LT.0.)TAU=0.
  STEP=(TAUM-TAU)/NI

*-----* Do 30 over time
  DO 30 I=1,NI+1
    TIM=FLOAT(I-1)*STEP
    TIME(I)=TFAC*(TAU+TIM)

```

```

      IF(TAUNU.GT.0.)THEN
        UP(I)=UPR*COF*SUM2(TIM,TE2,AL,BUF,50)
        UPAP(I)=UPR*EXP(-TIM/(BUF*GRNU(TNU,RHO)))
      ELSE
        UP(I)=4.*HSC*DIF*CII*SUM2(TIM,TE4,AL,BUF,50)/
1         R1**2*100.
        UPAP(I)=100.*HSC*DIF*CII/R1**2*(RHO**2-1.)
1         *EXP(-TIM/(BUF*GRNU(TNU,RHO)))/GRNU(TNU,RHO)
      ENDIF
      IF(TIM.LE.0.)THEN
        TUP(I)=UPR*TFAC*TAU
      ELSE
        IF(TAUNU.GT.0.)THEN
          TUP(I)=UPR*TFAC*TAU+COF*BUF*UPR*TFAC
1          *SUM1(TIM,TE1,AL,BUF,50)
          TUPAP(I)=UPR*TFAC*BUF*GRNU(TNU,RHO)*(1.-EXP(-TIM/
1          (BUF*GRNU(TNU,RHO)))) + UPR*TFAC*TAU
        ELSE
          TUP(I)=UPR*TFAC*TAU-4.*100.*TFAC*HSC*DIF*CII
1          *BUF*SUM1(TIM,TE3,AL,BUF,50)/R1**2
          TUPAP(I)=100.*HSC*DIF*CII/R1**2*(RHO**2-1.)*
1          TFAC*BUF*(1.-EXP(-TIM/(BUF*GRNU(TNU,RHO))))
        ENDIF
      ENDIF
30      CONTINUE
      RETURN
      END

```

```

*-----*
* Function GRNU                                     *
* Purpose: Calculation of G(nu,rho), (De Willigen & Van Noordwijk, 1987 *
*           page 130)                               *
*-----*
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time)      *
* name   type meaning                                units   class  *
*-----*-----*-----*-----*-----*
* TNU    R4    2*NU, NU dimensionless flux of water          -       I     *
* RHO    R4    Dimensionless radius soil cylinder           -       I     *
*-----*-----*-----*-----*-----*
* Subroutines called: none                                           *
* Functions called: none                                             *
* File usage: none                                                  *
*-----*

```

```

FUNCTION GRNU(TNU,RHO)
RHO2=RHO*RHO
IF(TNU.EQ.0.)THEN
  G1=(1.-3.*RHO2)/4.
  G2=RHO2**2*ALOG(RHO)/(RHO2-1.)
  GRNU=(G1+G2)/2.
  RETURN
ELSE
  GN1=(1.-RHO2)/2.
  GN2=RHO2*(RHO**TNU-1.)/TNU
  GN3=RHO2*(RHO**TNU-1.)*(TNU/2.+1.)/(TNU*
1  (RHO**(TNU+2.)-1.))
  GN4=(1.-RHO**(TNU+4.))*(TNU/2.+1.)/((TNU+4.)*
1  (RHO**(TNU+2.)-1.))
  GRNU=(GN1+GN2+GN3+GN4)/(TNU+2.)
ENDIF
RETURN
END

```

```

*-----*
* Subroutine ZEJY1                                     *
* Purpose: calculates the n-th root of:                 *
*            $Y(ORD+1, RHO*X)*J(ORD, X) - Y(ORD, X)*J(ORD+1, RHO*X)$  *
*           J, Y Bessel-functions of first kind, order ORD *
*           Solution by Newton-raphson iteration, first estimate as given *
*           in Abramowitz & Stegun , page 374, 9.5.33. *
* FORMAL PARAMETERS: (I=input, O=output, C=control, IN=init, T=time) *
* name   type meaning                                units  class *
*-----*-----*-----*-----*
* N      I4   rootnumber                               -      I   *
* TLIM   R4   maximum number of iterations             -      I   *
* EPS    R4   required accuracy                       -      I   *
* X      R4   the value of the root                   -      0   *
* IP     I4   Error indicator                         -      0   *
*
* Subroutines called: *
*   BESFRJ: calculates Bessel function J of fractional order *
*   BESFRY: calculates Bessel function Y of fractional order *
* Functions called: none *
* File usage: none *
*-----*

```

```

SUBROUTINE ZEJY1(X,N,RHO,ORD,TLIM,EPS,ISIG)
DIMENSION BJ(2),BY(2),BRJ(2),BRY(2)

```

```

DOUBLE PRECISION JNA,JNRA,JN1A,JN1RA,YNA,YNRA,YN1A,
$              YN1RA,FA,FAA
*   PRINT *, 'TLIM ', TLIM
   IP=0
   ORD1=ORD+1
   PI=3.141592654
   S=N
   X=(S-0.5)*PI/(RHO-1.)
   TEL=0.
1  SOL=X
   TEL=TEL+1
   IF(TEL.GT.TLIM)GO TO 5
   IF(SOL.LE.0.)GO TO 10
   RSOL=RHO*SOL
   CALL BESFRJ(SOL,ORD,ISIG,BJ)
   CALL BESFRY(SOL,ORD,ISIG,BY)
   CALL BESFRJ(RSOL,ORD,ISIG,BRJ)
   CALL BESFRY(RSOL,ORD,ISIG,BRY)
   JNA=BJ(1)
   JN1A=BJ(2)
   YNA=BY(1)
   YN1A=BY(2)
   JNRA=BRJ(1)
   JN1RA=BRJ(2)
   YNRA=BRY(1)
   YN1RA=BRY(2)

```



```

      DJN=JN1A+ORD/SOL*JNA
      DYN=YN1A+ORD/SOL*YN1A
      DJN1R=RHO*(JNRA-ORD1/RSOL*JN1RA)
      DYN1R=RHO*(YNRA-ORD1/RSOL*YN1RA)
      FA=JNA*YN1RA-JN1RA*YNA
*     PRINT *, 'TEL, SOL, FA ', TEL, SOL, FA
      FAA=YN1RA*DYN+JNA*DYN1R-JN1RA*DYN-YNA*DYN1R
      X=SOL-FA/FAA
      IF(ABS((SOL-X)/X).GT.EPS)GO TO 1
      RETURN
5     CONTINUE
      PRINT 100
      IP=2
      RETURN
10    PRINT 101, TEL, SOL
      IP=3
      RETURN

100   FORMAT(1H0, 'TOO MANY ITERATIONS IN ZEJY1')
101   FORMAT(1H0, 'AFTER', F5.0, 1X, 'ITERATION, NEGATIVE ARG: '
11PD15.5)

      END

```

```

*-----*
* Subroutine: BESFRJ                                     *
* Purpose: calculatesessel-functions first kind         *
* for argument x and (fractional) orders alph and alph+1 *
* *                                                     *
* FORMAL PARAMETERS: (I=input,O=output,C-control,IN=init,T=time) *
* name      type meaning                                units  class *
* -----*
* X         R4      argument of Besselfunction          -      I   *
* ALPH      R4      order of Besselfunction              -      I   *
* ISIG      R4      required significant digits          -      I   *
* BJ        R4      contains the values of J(ALPH,X), J(ALPH+1,X)      0   *
* *                                                     *
* Subroutines called:                                   *
*   BESJN from CERNLIB                                   *
* Functions called: none                                 *
* File usage: none                                       *
*-----*

```

```

SUBROUTINE BESFRJ(X,ALPH,ISIG,BJ)
DIMENSION BBJ(2),BJ(1)
C
  IF(ALPH.LT.0.)GO TO 5
  NNN=ALPH
  ALP=ALPH-NNN
  CALL BESJN(X,ALP,NNN,ISIG,BBJ)
  BJ(1)=BBJ(1)
  BJ(2)=BBJ(2)
  RETURN
5
  CONTINUE
  NNN=ALPH-1.
  ALP=ALPH-NNN
  CALL BESJN(X,ALP,NNN,ISIG,BBJ)
  BJ(1)=BBJ(2)
  BJ(2)=BBJ(1)
  RETURN
END

```

```

*-----*
* Subroutine BESFRY
* Purpose: calculates modified bessel-functions first kind
* for argument x and (fractional) orders alph and alph+1
*
*      X      R4      argument of Besselfunction      -      I
*      ALPH    R4      order of Besselfunction          -      I
*      ISIG    R4      required significant digits      -      I
*      BY      R4      contains the values of Y(ALPH,X), Y(ALPH+1,X)      0
*
* Subroutines called:
*   BESFRJ
* Functions called: none
* File usage: none
*-----*

```

```

SUBROUTINE BESFRY(X,ALPH,ISIG,BY)
DIMENSION BY(1),BBJ(2),BBMJ(2)
PI=3.1415926535
CO=COS(ALPH*PI)
SI=SIN(ALPH*PI)
ALP=-ALPH
CALL BESFRJ(X,ALP,ISIG,BBMJ)
CALL BESFRJ(X,ALPH,ISIG,BBJ)
BY(1)=(BBJ(1)*CO-BBMJ(1))/SI
BY(2)=(2./(PI*X)-BBJ(2)*BY(1))/BBJ(1)
1 CONTINUE
RETURN
END

```

APPENDIX II. Numerical solution of radial flow of water to a plant root.

Background

The program solves the following partial differential equation,

$$\frac{\partial \theta}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} D_w \frac{\partial \theta}{\partial r} \quad (\text{AII-1})$$

with boundary conditions:

$$r = \rho, \quad \frac{\partial \theta}{\partial r} = 0 \quad (\text{AII-2})$$

and either:

$$r = 1, \quad \left(D_w \frac{\partial \theta}{\partial r} \right) = \text{constant} = q \quad (\text{AII-3a})$$

or:

$$r = 1, \quad \theta = \text{constant} = \theta_{rs} \quad (\text{AII-3b})$$

The initial condition is simply :

$$t = 0, \quad \theta = \text{constant} = \theta_i \quad (\text{AII-4})$$

The meaning of the symbols can be found in table 1 in the main text. Equation (AII-1) is Richard's equation in cylindrical coordinates.

Before discretizing the partial differential equation (AII-1), the hollow cylinder with inner radius 1 and outer radius ρ , is transformed to a rectangle by the transformation:

$$x = \ln r \quad (\text{AII-5})$$

This transforms (AII-1)-(AII-3) into resp.:

$$e^{2x} \frac{\partial \theta}{\partial t} - \frac{\partial}{\partial x} D_w \frac{\partial \theta}{\partial x} \quad (\text{AII-6})$$

$$x = \ln \rho, \quad \frac{\partial \theta}{\partial x} = 0, \quad (\text{AII-7})$$

$$x = 0, \quad \frac{\partial \theta}{\partial x} = q \quad (\text{AII-8a})$$

and

$$x = 0, \quad \theta = \theta_{rs}$$

(AII-8b)

Equation (AII-6) is discretized by dividing the region $0 < x < \ln\rho$ into a number of control-volumes and integrating of (AII-6) over the control-columne and a finite time-step Δt (Patankar, 1980) following a complete implicit scheme. This leads to a set of n equations in the n unknown θ , where n is the number of control volumes. These equations have the form:

$$a_i \theta_i = b_i \theta_{i+1} + c_i \theta_{i-1} + d_i$$

(AII-9)

where

$$b_i = \frac{\overline{D_i}}{\Delta x}, \quad c_i = \frac{\overline{D_{i-1}}}{\Delta x},$$

$$a_i = b_i + c_i + \sinh(\Delta x) \frac{e^{2(i-1)\Delta x}}{\Delta t}, \quad d_i = \sinh(\Delta x) \frac{e^{2(i-1)\Delta x}}{\Delta t} \theta_i^0$$

Δx is the thickness of the control-volumes, Δt the time-step, D_i and D_{i-1} the average diffusivities at the boundaries of control-volume i and $i+1$, resp $i-1$ and i . It is to be understood that all values of θ are the new unknown values at time $t+\Delta t$ except where the superscript 0 is used. The coefficients a, b, c and have special values at the boundaries, where $i=1$ resp $i=n$. For $i=1$ ($x=0$), if condition of constant flux (AII-8a) is used:

$$a_1 = \frac{(e^{\Delta x}-1)}{2\Delta t} + \frac{\overline{D_1}}{\Delta x}, \quad b_1 = \frac{\overline{D_1}}{\Delta x}$$

$$c_1 = 0, \quad d_1 = -q + \frac{(e^{\Delta x}-1)}{2\Delta t} \theta_1^0,$$

whereas when for constant watercontent (AII-8b):

$$a_1 = 1, \quad b_1 = 0, \quad c_1 = 0, \quad d_1 = \theta_{rs}.$$

For $i=n$ ($x=\ln\rho$)

$$a_n = \frac{(\rho^2 - e^{2(n-1)\Delta x - \Delta x})}{2\Delta t}, \quad b_n = 0$$

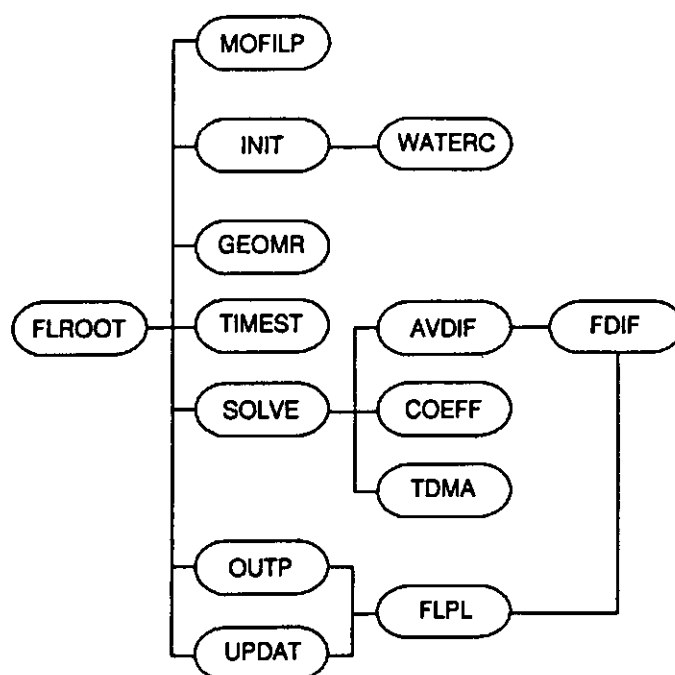
$$c_n = \frac{\overline{D_{n-1}}}{\Delta x}, \quad d_n = \frac{(\rho^2 - e^{(n-1)\Delta x - \Delta x})}{2\Delta t} \theta_n^0$$

The solution of the discretization equations (AII-9) is found by the TDMA algorithm (Patankar, 1980).

Program

The relation between the subroutines is given in the diagram in Figure AII-1. The core of the program is formed by the subroutine SOLVE wherein the discretization equations are solved. Due to the nonlinear relation between the diffusivity and the water content the solution is found by iteration. If necessary underrelaxation can be used to avoid divergence (Patankar, 1980, Ch 4. page 67).

Relational diagram of subroutines in FLROOT



The relation between diffusivity and water content is as proposed by Van Genuchten (1980):

$$D = K_s \frac{W^l}{(\theta_{sat} - \theta_r) \alpha n} \left(w^{-\frac{1}{m}} - 1 \right)^{(-m)} \left[1 - \left(1 - w^{\frac{1}{m}} \right)^m \right]^2 \quad (\text{AII-10})$$

where

$$W = \frac{\theta - \theta_r}{\theta_{sat} - \theta_r}, \quad m = 1 - \frac{1}{n}$$

This is calculated in the function FDIF, and is used in the function FLPL which calculates the integral give in (11). The numerical integration is performed by the function GAUSS (not shown) which is taken from CERNLIB Lindelof, 1981).

```

*-----*
* Program FLROOT *
* Purpose : Calculation of flow of water towards a root. *
*           The geometry is a hollow cylinder representing the soil around *
*           the root. Boundary conditions are: constant flux, or constant *
*           water-content at the root surface (the inner cylinder) and *
*           zero-flux at the outer cylinder. The partial differential *
*           equation is solved by completely implicit finite difference *
*           scheme, as described in S.V. Patankar, 1980, Numerical heat *
*           transfer and fluid flow. *
*           The flow is also calculated with an analytical function, *
*           based on the steady-rate approximation (De Willigen and *
*           Van Noordwijk, 1987, Roots, plant production and nutrient use *
*           efficiency page 149, (9.73)). *
*           *
* The mutual relations between matric potential, water content, *
* and hydraulic conductivity are given by Van Genuchten functions. *
*           *
* SUBROUTINES called: *
*   MOFILP: organizes input *
*   INIT: initializes watercontent *
*   GEOMR: calculates geometry, thickness control-volumes etc. *
*   SOLVE: solves the discretization equations *
*   UPDAT: updates watercontent, calculate totals, averages, etc. *
*   OUTP: organizes the output *
*           *
* FILE usage: *
*   1. input from screen (format: soilname.DAT), unit 40, *
*      contains soil and root data (I) *
*   2. CONTR.DAT, unit 40, contains data that control boundary *
*      conditions, iteration, relaxation (I) *
*   3. soilname.PET, unit 41, main outputfile (O) *
*   4. soilname.PLO, unit 48, plotfile with data (O) *
*           *
*-----*

```

```

DIMENSION G(30),C(30),WCN(30),DIFDN(30)
DIMENSION A(30),X(30),B(30),D(30),WCOL(30)
DIMENSION USTR(30),WCSTR(30),DW(30)

```

```

REAL KS,M,N,L
REAL U(30),R(30),LRV
REAL WC(30),DWCDT(30),DIFD(30)
CHARACTER*20 NAME,INP,OUTF
LOGICAL MODE

```

```

COMMON /FDIF1 / WCSAT,WCR,M,N,L,ALPH,KS

```

```

DATA FLB/1./

```

```

*----- INITIAL -----*

```



```

PI=ATAN(1.)*4.
TWOPI=2.*PI

```

```

*----- input
PRINT *, 'SOILNAME?'
READ(*,100) NAME

```

```

*----- File with soil and root-data is opened
OPEN (UNIT=40,FILE=NAME)

```

```

*----- Outputfile is opened
I = INDEX (NAME, '.')
IF (I.EQ.0) I = INDEX (NAME, ' ')
NAME(I:I+3) = '.PET'
OPEN (UNIT=41,FILE=NAME)

```

```

*----- Plotfile is opened
NAME(I:I+3) = '.PLO'
OPEN(UNIT=48,FILE=NAME)

```

```

*----- Reading of soil and root data
CALL MOFILP(40)
READ(40,100) NAME
CALL MOFILP(40)
READ(40,*) WCSAT,WCR,WCMIN,WCREF,PLIM,PMIN
PRINT *, 'WCSAT,WCR,WCMIN,WCREF,PLIM ', WCSAT,WCR,WCMIN,WCREF,PLIM
CALL MOFILP(40)
READ(40,*) KS,N,L,ALPH
M=1.-1./N
CALL MOFILP(40)
READ(40,*) LRV,R0,HSC
CALL MOFILP(40)
READ(40,*) EVAP
CALL MOFILP(40)
READ(40,*) WCI
CALL MOFILP(40)
READ(40,*) IR
CLOSE(40)

```

```

*----- SOILNAME.DAT is closed

```

```

*----- CONTR.DAT is opened
OPEN(FILE='CONTR.DAT',UNIT=40)

```

```

*----- reading control data

```

```

CALL MOFILP(40)
READ (40,*) TFAC

```

```

*----- maximum change watercontent

```

```

*----- over time-step

```

```

CALL MOFILP(40)
READ (40,*) CHMAX

```

```

*----- iteration tolerance

```

```

CALL MOFILP(40)

```

```

      READ (40,*) EPS
*----- relaxation factor
      CALL MOFILP(40)
      READ (40,*) RELF
*----- CWRS < 0 , watercontent at root surface
*----- constant
      CALL MOFILP(40)
      READ (40,*) CWRS
*----- read waterpotential root
*----- surface
      IF(CWRS.LT.0.)THEN
        CALL MOFILP(40)
        READ (40,*) PRS
        FLB=-1.
      ELSE
        ENDIF
*----- Close CONTR.DAT
      CLOSE(40)

*----- End input
*----- Initialisation
      CALL INIT(IR,LRV,HSC,RO,WCI,PLIM,EVAP,FLB,PRS,
1          R1,SUMWI,RHO,ETA,WCLIM,QT,RAT,WC,WAPP)

*----- Reading time data from screen
      TMAX=SUMWI/(PI*R1**2*EVAP)
      PRINT *, 'MAXIMUM EXTRACTION TIME IN DAYS ',TMAX
      PRINT *, 'GIVE FINTIM IN DAYS'
      READ *,FINTIM
      PRINT *, 'PRINT-INTERVAL IN DAYS'
      READ *,PRDEL

*----- Geometry
      CALL GEOMR(IR,RHO,X,R,DX,DX2)

      PRDELT=PRDEL*RAT
      IP=0
      T=0
      WRITE(41,*) 'FINTIM,DELT,DT ',FINTIM,DELT,DT

      DELT=.1
      FIT=0
      TRPAR=1.
      WAPP=WCI

*----- DYNAMIC -----*

10      CONTINUE

      IF(WC(1).LE.WCLIM.AND.FLB.GT.0.)THEN
        FLB=-1.

```

```

        WRITE(41,*) 'TIME = ',TIME,'    WC(1).LE.WCLIM'
        PRINT 101,TIME,DELT
        PRINT 102,(WC(K),K=1,IR)
        CALL OUTP(IR,R,RO,HSC,R1,T,TIME,DELT,WCN,WC,DWCDT,DIFD,
1          BAL,RUPW,RUPWSR,CUPW,CUPWSR,WCAV,WCAPP)
        ENDIF

*----- Check if time exceeds fintim
        IF(TIME.GE.FINTIM)GO TO 20

*----- Check if output should be written
        IF(TIME.GE.(IP*PRDEL))THEN
            IP=IP+1
            CALL OUTP(IR,R,RO,HSC,R1,T,TIME,DELT,WCN,WC,DWCDT,DIFD,
1          BAL,RUPW,RUPWSR,CUPW,CUPWSR,WCAV,WCAPP)
            ENDIF

        CALL SOLVE(IR,WC,WCN,DELT,DX,RHO,QT,FLB,RELF,EPS,WCLIM,
1          DIFD)

        CALL UPDAT(IR,WC,WCN,WCLIM,R,RO,R1,HSC,DELT,T,
1          DWCDT,RUPW,RUPWSR,CUPWSR,CUPW,BAL,WCAV,WCAPP)

        TIME=T*(RO*RO)

        CALL TIMEST(DELT,FLB,TFAC,CHMAX,WC,DWCDT,PRDEL)

        GO TO 10

20      CONTINUE
        WRITE(41,*) ' TIME .GE. FINTIM '
        CALL OUTP(IR,R,RO,HSC,R1,T,TIME,DELT,WCN,WC,DWCDT,DIFD,
1          BAL,RUPW,RUPWSR,CUPW,CUPWSR,WCAV,WCAPP)
        STOP

100     FORMAT(A20)
101     FORMAT(1H0,'TIME ='1PE15.5,1X,'DELT ='1PE15.5)
102     FORMAT(1H0,/13X,'WC'/(1PE15.5))

        END

```

```

*-----*
* Subroutine INIT *
* Purpose: Initialisation of watercontent, calculation of parameters *
* FORMAL PARAMETERS: (I=input,0=output,C-control,IN-init,T-time) *
* name type meaning units class *
*-----*
* LRV R4 Root length density cm/cm3 I *
* HSC R4 Root lenght cm I *
* RO R4 Root radius cm I *
* WCI R4 Initial water content - I *
* PLIM R4 Limiting value matric potential cm I *
* EVAP R4 Required transpiration cm/day I *
* FLB R4 Parameter that controls boundary condition I *
* at root surface. FLB>0 constant flux, *
* FLB<0 constant watercontent *
* PRS R4 Matric potential at root surface cm I *
* R1 R4 Radius soil cylinder cm 0 *
* RHO R4 Dimensionless radius soil cylinder - 0 *
* SUMWI R4 Initial total amount of water in soil cm3 0 *
* ETA R4 Dimensionless root lenght - 0 *
* WCLIM R4 limiting value water content - 0 *
* QT R4 Required uptake rate of water by root cm2/day 0 *
* WC R4 Water content - 0 *
* WCAPP R4 Water content calculated by steady-rate - 0 *
* approximation *
* Subroutines called: none *
* Functions called: *
* WATERC: calculates water content as a function of matric potential *
* File usage: soilname.PET *
*-----*

```

```

SUBROUTINE INIT(IR,LRV,HSC,RO,WCI,PLIM,EVAP,FLB,PRS,
1          R1,SUMWI,RHO,ETA,WCLIM,QT,RAT,WC,WCAPP)
  DIMENSION WC(30)
  REAL M,N,L,KS,LRV
  COMMON /FDIF1 / WCSAT,WCR,M,N,L,ALPH,KS

  PI=4.*ATAN(1.)
  R1=1./SQRT(PI*LRV)
  SUMWI=PI*(R1*R1-RO*RO)*HSC*WCI
  RHO=R1/RO
  ETA=HSC/RO
  WCLIM=WATERC(PLIM,WCSAT,WCR,N,ALPH)
  QT=RHO**2/(2.*ETA)*EVAP*RO
  RAT=1./(RO*RO)

```

```

*-----* initialisation OF WATER CONTENT
  DO 30 K=2,IR+1
    WC(K)=WCI

```

```

30      CONTINUE
        IF (FLB.GT.0.) THEN
            WC(1)=WCI
        ELSE
            WC(1)=WATERC(PRS,WCSAT,WCR,N,ALPH)
        ENDIF
        WCAPP=WCI

*----- initial output
        WRITE(41,100) LRV,EVAP,RHO,ALPH,QT,RAT
        PRINT      100,LRV,EVAP,RHO,ALPH,QT,RAT
        PRINT 101,SUMWI
        WRITE(41,101) SUMWI
        RETURN

100      FORMAT(1X,/,1X,'ROOT-DENSITY CM-2:'F5.1/
1         1X,'EVAPOTRANSPIRATION CM/DAY :'F6.2/
2         1X,'RHO ;'1PE15.5/
3         1X,'ALPH :'1PE15.5/1X,
4         1X,'DIMENSIONLESS UPTAKE QT:'1PE15.5/
5         1X,'RATIO DIMENSIONLESS TIME AND REAL TIME:'1PE15.5)
101      FORMAT(1X,'SUMWI-'1PE15.5)

        END

```

```

*-----*
* Subroutine: SOLVE                                     *
* Purpose: construction of coefficient-matrix of discretized equations *
*         and solving the equations by TDMA             *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time) *
* name      type meaning                                units  class *
*-----*-----*-----*-----*-----*
* WC        R4    Water content                        -      I    *
* WCN       R4    New values of water content          -      I,0  *
* DELT      R4    Time step in scaled units            day/cm2 I    *
* DX        R4    Thickness control-volume             -      I    *
* RHO       R4    Dimensionless radius soil cylinder   -      I    *
* QT        R4    Uptake rate of water by root         cm2/day I    *
* FLB       R4    Parameter that controls boundary condition *
*               at root surface. FLB>0 constant flux,    *
*               FLB<0 constant watercontent              *
* RELF      R4    Relaxation factor                    -      I    *
* EPS       R4    Convergence criterion for iteration   -      I    *
* DIFD      R4    Average diffusivity at face control volume -      0    *
* WCLIM     R4    limiting value water content          -      0    *
*-----*
* Subroutines called:                                  *
*   COEFF: calculates coefficients discretization equations *
*   TDMA : solves discrization equations                 *
*-----*
* Functions called:                                    *
*   AVDIF: calculates average diffusivity at interface    *
*           two control-volumes                          *
* File usage: none                                       *
*-----*

```

```

      SUBROUTINE SOLVE(IR,WC,WCN,DELT,DX,RHO,QT,FLB,RELF,EPS,WCLIM,
1          DIFD)
      DIMENSION WC(30),WCN(30)
      DIMENSION WCOL(30),DIFD(30),A(30),B(30),C(30),D(30),DIFDN(30)

10      CONTINUE
      ----- average diffusivities are calculated
      ----- old values of WC stored in WCOL
      DO 20 K=1,IR-1
          DIFD(K)=AVDIF(WC(K),WC(K+1),.FALSE.)
          WCOL(K)=WC(K)
20      CONTINUE
      WCOL(IR)=WC(IR)

      ----- tentative new values of WC (WCN) calculated
      ----- no relaxation
1      CALL COEFF(IR,A,B,C,D,WC,DIFD,1.,DX,RHO,DELT,QT,FLB,WC(1),
          WCOL,RELF,0)
      CALL TDMA(IR,A,B,C,D,WCN)

```

```

*----- iterative search for better new values of WC
      DO 50 IT=1,10
        IF(WCN(1).LT.0.)GO TO 60
        DO 30 K=1,IR-1
          TRPAR=1.
          IF(WCN(K).LT.WCLIM)THEN
            TRPAR=-1.
          ENDIF
          DIFDN(K)=AVDIF(WCN(K),WCN(K+1),.FALSE.)
30      CONTINUE
*----- criterion of convergence is relative
*----- difference between consecutive values of
*----- diffusivity at first or second gridpoint
      DIFCRT=(DIFDN(1)-DIFD(1))/DIFD(1)
      IF(FLB.LT.0.)DIFCRT=(DIFDN(2)-DIFD(2))/DIFD(2)
      IF(ABS(DIFCRT).LT.EPS)THEN
        GO TO 70
      ELSE
1      CALL COEFF(IR,A,B,C,D,WC,DIFDN,1.,DX,RHO,DELT,QT,FLB,
              WC(1),WCOL,RELF,IT)
      CALL TDMA(IR,A,B,C,D,WCN)
      DO 40 K=1,IR
        TRPAR=1.
        IF(WCN(K).LT.WCLIM)THEN
          TRPAR=-1.
        ENDIF
        DIFD(K)=DIFDN(K)
        WCOL(K)=WCN(K)
40      CONTINUE
      ENDIF
50      CONTINUE
60      DELT=DELT/2.
      GO TO 10

*----- end of iteration
70      CONTINUE

      RETURN
      END

```

```

*-----*
* Function FLPL *
* Purpose: Calculation of matric flux potential as integral of diffusivity*
*           over watercontent *
* *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time) *
* name   type meaning                                units   class *
* -----*
* WC      R4   water content                          ml/cm3   I   *
* WCSAT   R4   Watercontent at saturation             ml/cm3   I   *
* N        R4   parameter from conductivity-watercontent *
*           relation *
* ALPH     R4   parameter                             cm-1     I   *
* WCR      R4   residual water content                 ml/cm3   I   *
* KS       R4   saturated conductivity                 cm/day   I   *
* *
* Subroutines called: none *
* *
* Functions called : *
*   GAUSS: a function from CERNLIB which performs numerical *
*           integration according to Gauss' method. *
*   FDIF: calculates diffusivity as a function of water content. *
* *
* File usage: none *
*-----*

```

```

REAL FUNCTION FLPL(WC)
REAL KS,M,N,L
COMMON /FDIF1/ WCSAT,WCR,M,N,L,ALPH,KS
EXTERNAL FDIF

FLPL=GAUSS(FDIF,WC,0.99*WCSAT,.001)

RETURN
END

```



```

*-----*
* FUNCTION WATERC                                     *
* Purpose : Calculation of watercontent by hydraulic head Van Genuchten *
*           function.                                *
* FORMAL PARAMETERS: (I=input,0-output,C-control,IN-init,T-time)      *
* name   type meaning                                units   class *
*-----*-----*-----*-----*-----*
* PRES   R4   hydraulic head                        cm       I   *
* WCSAT  R4   Watercontent at saturation             ml/cm3    I   *
* N      R4   parameter from conductivity-watercontent -       I   *
*           relation                                *
* ALPH   R4   parameter                             cm-1     I   *
* WCR    R4   residual water content                 ml/cm3    I   *
* WATERC R4   watercontent                          ml/cm3    0   *
*-----*
* Subroutines/functions called: none.                    *
*-----*
* File usage: none                                       *
*-----*

```

```

FUNCTION WATERC(PRES,WCSAT,WCR,N,ALPH)
REAL M,N
M=1.-1./N
IF(PRES.LE.0.)THEN
  TRPAR=-1
ENDIF
HELP=(1.+(ALPH*PRES)**N)
IF(HELP.LE.0.)THEN
  TRPAR=-1
ELSE
  ENDIF
WATERC=(WCSAT-WCR)*(1.+(ALPH*PRES)**N)**(-M)+WCR
RETURN
END

```

```

*-----*
* Function FDIF                                     *
* Purpose: Calculation of diffusivity from watercontent *
* FORMAL PARAMETERS: (I=input, O=output, C=control, IN=init, T=time) *
* name      type meaning                            units  class *
* -----*
* WCSAT    R4    Watercontent at saturation          ml/cm3   I    *
* N         R4    parameter from conductivity-watercontent -      I    *
*           relation                                *
* ALPH      R4    parameter                          cm-1     I    *
* WCR       R4    residual water content             ml/cm3   I    *
* FDIF      R4    Diffusivity                       cm2/day  *
*
* SUBROUTINES called: none                          *
* FUNCTIONS called: none                            *
* FILE usage:none                                   *
*-----*

```

```

      FUNCTION FDIF(WC)
      REAL KS,M,N,L
      COMMON /FDIF1/ WCSAT,WCR,M,N,L,ALPH,KS

      W=(WC-WCR)/(WCSAT-WCR)
      M=1.-1./N
      TRPAR=1.
      IF(W.LT.0.)THEN
        TRPAR=-1.
      ENDIF
      WL=W**(-1./M)
      TRPAR=1
      IF(WL.LE.1.)THEN
        TRPAR=-1
      ENDIF
      FDIF=KS*W**L/((WCSAT-WCR)*ALPH*N)*(WL-1.)**(-M)*
1      (1.-(1.-W**(1./M))**M)**2
      RETURN
      END
      FUNCTION FG(R)
      FG=0.5*((1-3.*R**2)/4.+R**4*ALOG(R)/(R**2-1))
      RETURN
      END

```

```

*-----*
* Subroutine TIMEST                                     *
* Purpose: calculation of time step DELT               *
*-----*
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time) *
* name   type meaning                                units  class *
*-----*-----*-----*
* DELT   R4    timestep in scaled units              day/cm2 I,O  *
* TFAC   R4    multiplying factor, if possible DELT is      I      *
*         increased by TFAC                               *
* CHMAX  R4    permitted maximum relative change in        -      I      *
*         watercontent                                     *
* WC     R4    watercontent                                I      *
* DWCDT  R4    rate of change of WC                     cm2/day I  *
* PRDELTA R4    print-interval in scaled units            day/cm2 I  *
*-----*
* Subroutines/Functions called: none                   *
* FILE usage: none                                     *
*-----*

```

```

SUBROUTINE TIMEST(DELTA,FLB,TFAC,CHMAX,WC,DWCDT,PRDELTA)
DIMENSION WC(30),DWCDT(30)

```

```

IF(FLB.GT.0.)THEN
  DCH=CHMAX*WC(1)/ABS(DWCDT(1))
ELSE
  DCH=CHMAX*WC(2)/ABS(DWCDT(2))
ENDIF
DELTA2=DELTA*TFAC
DELTA=AMIN1(DCH,PRDELTA,DELTA2)

```

```

RETURN
END

```

```

*-----*
* Subroutine: UPDAT *
* Purpose: Updating of watercontent, time, total amount of water in soil, *
*          decrease of total water, transpiration by steady-rate *
*          approximation *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time) *
* name type meaning units class *
*-----*
* R R4 Dimensionless radial coordinate - I *
* R0 R4 Radius root cm I *
* HSC R4 Root length cm I *
* R1 R4 Radius soil cylinder cm I *
* WC R4 Water content - I,0 *
* WCN R4 New values of water content - I *
* DWCDT R4 Rate of change of water content cm2/day I *
* DELT R4 timestep in scaled units day/cm2 I *
* RHO R4 Dimensionless radius soil cylinder - I *
* WCLIM R4 water content at root surface - I *
* RUPW R4 Rate of uptake of water cm/day 0 *
* CUPW R4 Cumulative water uptake cm 0 *
* R As RUPW and CUPW but calculated with cm/day 0 *
* CUPWSR R4 steady-rate approximation cm 0 *
* BAL R4 Balance of water in soil cm 0 *
* WCAPP R4 Average water content calculated by steady- - 0 *
*          rate approximation *
* WCAV R4 Average water content - 0 *
*
* Subroutines called: none. *
*
* Functions called: *
* FLPL: calculates matric flux potential as a function of *
*        water content *
*-----*

```

```

SUBROUTINE UPDAT(IR,WC,WCN,WCLIM,R,R0,R1,HSC,DELT,T,
1 DWCDT,RUPW,RUPWSR,CUPWSR,CUPW,BAL,WCAV,WCAPP)

```

```

DIMENSION WC(30),WCN(30),DWCDT(30),R(30),USTR(30)
LOGICAL INIT
DATA INIT/.FALSE./

```

```

IF(.NOT.INIT) THEN
  RHO=R1/R0
  ETA=HSC/R0
  PI=4.*ATAN(1.)
  INIT=.TRUE.
  SUMWI=(R1*R1-R0*R0)*HSC*WC(2)/R1**2
ENDIF

```

```

*----- calculation of DWC/DT
      DO 10 K=1,IR
        DWCDT(K)=(WCN(K)-WC(K))/DELT
10    CONTINUE

*----- SUMW total water in soil cylinder cm
*----- RUPW rate of decrease of water cm/day
      SUMW=0.
      RUPW=0.
      DO 20 K=1,IR-1
        SUMW=SUMW+
1      (R(K+1)-R(K))*(R(K+1)*WC(K+1)+R(K)*WC(K))/2.
        RUPW=RUPW+
1      (R(K+1)-R(K))*(R(K+1)*DWCDT(K+1)+R(K)*DWCDT(K))/2.
20    CONTINUE
      SUMW=2.*HSC*R0**2*SUMW/R1**2
      RUPW=-2.*HSC*RUPW/R1**2
      BAL=SUMW+CUPW-SUMWI

*----- WCAV average water content
      WCAV=SUMW*R1**2/(HSC*(R1**2-R0**2))
      USTR(1)=FLPL(WC(1))
      UAVAPP=FLPL(WCAPP)

*----- RUPWSR water uptake according to steady-rate
*----- approximation cm/day
      RUPWSR=2.*HSC/R1**2*(USTR(1)-UAVAPP)*(RHO**2-1.)/(2.*FG(RHO))

*-----
      IF(WCN(1).LE.WCLIM.AND. WC(1).GT.WCLIM)THEN
        DELT=AMIN1(DELT,(WCLIM-WC(1))/DWCDT(1))
        TRPAR=-1.
      ENDIF

*----- Updating of WC
      DO 30 K=1,IR
        WC(K)=WC(K)+DWCDT(K)*DELT
        TPAR=1.
        IF(WC(K).LT.WCLIM)THEN
          TRPAR=-1.
        ENDIF
30    CONTINUE

      T=T+DELT

      CUPW=CUPW+RUPW*DELT*R0**2
      CUPWSR=CUPWSR+RUPWSR*DELT*R0**2
      WCAPP=WCAPP-RUPWSR*DELT*R0**2*R1**2/(HSC*(R1**2-R0**2))
      RETURN
      END

```

```

*-----*
* Subroutine GEOMR                                     *
* Purpose: calculation of position of gridpoints both in transformed and *
*          untransformed coordinates                     *
* Note: Gridpoints equidistant in transformed region, distances between *
* gridpoints geometrically increasing in untransformed cylindrical region.*
*-----*
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time)      *
* name   type meaning                                     units   class *
*-----*-----*-----*-----*-----*
* IR      I4   Number of gridpoints                        -         I   *
* RHO      R4   Dimensionless radius soil cylinder         -         I   *
* R        R4   Radial coordinate gridpoint                -         0   *
* X        R4   Coordinate of gridpoint in transformed region: -      0   *
*          X = Ln(R)                                       *
* DX       R4   Distance between gridpoints in transformed region *
*-----*
* Subroutine/Finctions called: none *
*-----*
* File usage: Coordinates gridpoints writen to file soilname.PET *
*-----*

```

```

SUBROUTINE GEOMR(IR,RHO,X,R,DX,DX2)
DIMENSION X(30),R(30)

DX=ALOG(RHO)/(IR-1)
DX2=DX*DX
R(1)=1.
X(1)=0.
DO 10 K=2,IR
    X(K)=X(K-1)+DX
    R(K)=EXP(X(K))
10  CONTINUE

WRITE(41,100) IR,DR
PRINT 100,IR,DR

WRITE(41,101) (R(K),K=1,IR)
PRINT 101,(R(K),K=1,IR)

RETURN

100  FORMAT(1H0,I3,1X,'POINTS IN R-DIRECTION'/
3/1X,'DR='1PE15.5)
101  FORMAT(1H0,'R='1P5E15.5)

END

```

```

*-----*
* Function: AVDIF                                     *
* Purpose: calculates harmonic or arithmetic average of diffusivities, *
*           with equal weights                         *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time)    *
* name  type meaning                                units  class *
*-----*-----*-----*-----*
* X1,X2  R4   dummies, representing watercontent        -      I   *
* MODE   L    If .true. harmonic average, else arithmetic *
*-----*-----*-----*-----*
* Subroutines called: none *
*-----*
* Functions called: *
*   FDIF: calculates diffusivity as a function of water content *
*-----*
* File usage: none *
*-----*

```

```

FUNCTION AVDIF(X1,X2,MODE)
  LOGICAL MODE
  D1=FDIF(X1)
  D2=FDIF(X2)
  IF(MODE) THEN
    AVDIF=2*D1*D2/(D1+D2)
  ELSE
    AVDIF=(D1+D2)/2.
  ENDIF
  RETURN
END

```

```

*-----*
* Subroutine COEFF                                     *
* Purpose: calculation of coefficients of the discretization equations. *
*       These are of the form:                        *
*        $A(I)*T(I) - B(I)*T(I+1) + C(I)*T(I-1) + D(I)$ , where  $T(I)$  is the *
*       value of the dependent variable at gridpoint I. *
*-----*
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time) *
* name   type meaning                                     units   class *
*-----*-----*-----*-----*-----*
*  N      I4  Number of gridpoints                        -        I   *
*  A,B,C,D R4  Coefficients                               -        0   *
*  T      R4  Dummy denoting the dependent variable      -        I   *
*  FM      R4  If FM=1 scheme completely implicit, FM=0   -        I   *
*              scheme completely explicit                -        I   *
*  DX      R4  distance between gridpoints                -        I   *
*  RHO      R4  dimensionless radius soil cylinder        -        I   *
*  DT      R4  timestep                                    -        I   *
*  Q        R4  uptake rate                               -        I   *
*  FLB      R4  Parameter that controls boundary condition -        I   *
*              at root surface. FLB>0 constant flux,     -        I   *
*              FLB<0 constant watercontent               -        I   *
*  WCLIM    R4  water content at root surface              -        I   *
*  TO       R4  Values of T at preceding time-step        -        I   *
*  RELF     R4  Relaxation factor                          -        I   *
*  IT       R4  Controls relaxation, if IT >1 relaxation  -        I   *
*-----*
* Subroutines/functions called: none *
*-----*
* File usage: none *
*-----*

```

```

SUBROUTINE COEFF(N,A,B,C,D,T,DIF,FM,DX,RHO,DT,Q,FLB,WCLIM,
1              TO,RELF,IT)
  DIMENSION A(30),B(30),C(30),D(30),T(30),TO(30),DIF(30)
  EMFM=1.-FM
  BETA=(EXP(DX)-EXP(-DX))/2.

  DO 5 I=2,N-1
    AE=DIF(I)/DX
    AW=DIF(I-1)/DX
    AOP=BETA*EXP(2.*(FLOAT(I)-1.)*DX)/DT
    AI=(FM*AE+FM*AW+AOP)

    B(I)=FM*AE
    C(I)=FM*AW
    DI=AE*EMFM*T(I+1) + AW*EMFM*T(I-1) +
1      (AOP-EMFM*AE-EMFM*AW)*T(I)

```



```

      IF(IT.LE.1)THEN
        A(I)=AI
        D(I)=DI
      ELSE
        A(I)=AI/RELF
        D(I)=DI+(1.-RELF)*A(I)*TO(I)
      ENDIF

```

5 CONTINUE

```

      IF(FLB.GT.0.)THEN
        A1=((EXP(DX)-1.)/(2.*DT)+DIF(1)*FM/DX)
        B(1)=DIF(1)*FM/DX
        C(1)=0.
        D1=DIF(1)*EMFM*(T(2)-T(1))/DX - Q +
1         (EXP(DX)-1.)/(2.*DT)*T(1)

```

```

      IF(IT.LE.1)THEN
        A(1)=A1
        D(1)=D1
      ELSE
        A(1)=A1/RELF
        D(1)=D1+(1.-RELF)*A(1)*TO(1)
      ENDIF

```

```

    ELSE
      A(1)=1.
      B(1)=0.
      C(1)=0.
      D(1)=WCLIM
    ENDIF

```

```

    AN=((RHO**2-EXP(2.*FLOAT(N-1)*DX-DX))/(2.*DT)+
1     DIF(N-1)*FM/DX)
    B(N)=0.
    C(N)=DIF(N-1)*FM/DX
    DN=DIF(N-1)*EMFM*(T(N)-T(N-1))/DX +
1     (RHO**2-EXP(2.*FLOAT(N-1)*DX-DX))/(2.*DT)*T(N)

```

```

    IF(IT.LE.1)THEN
      A(N)=AN
      D(N)=DN
    ELSE
      A(N)=AN/RELF
      D(N)=DN+(1.-RELF)*A(N)*TO(N)
    ENDIF

```

```

  RETURN
END

```

```

*-----*
* Subroutine TDMA                                     *
* Purpose: solves the discretization equations        *
*                                                     *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time) *
* name      type meaning                               units  class *
* -----*-----*-----*-----*-----*-----*
*  N        I4   Number of gridpoints                  -      I   *
*  A,B,C,D  R4   Coefficients                          -      I   *
*  TE       R4   Dummy denoting the dependent variable  -      O   *
*                                                     *
* Subroutines/Functions called: none                 *
*                                                     *
* File usage: none                                   *
*-----*

```

```

SUBROUTINE TDMA(N,A,B,C,D,TE)
  DIMENSION A(30),B(30),C(30),D(30),TE(30)
  REAL P(50),Q(50)
  P(1)=B(1)/A(1)
  Q(1)=D(1)/A(1)
  DO 5 I=2,N
    DENOM=A(I)-C(I)*P(I-1)
    P(I)=B(I)/DENOM
    Q(I)=(D(I)+C(I)*Q(I-1))/DENOM
5  CONTINUE
  TE(N)=Q(N)
  DO 10 I=N-1,1,-1
    TE(I)=P(I)*TE(I+1)+Q(I)
10 CONTINUE
  RETURN
END

```

```

*-----*
* Subroutine OUTP                                     *
* Purpose: organizes output                           *
*                                                     *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time) *
* name      type meaning                               units  class *
*-----*-----*-----*-----*-----*
* IR        I4    Number of gridpoints                 -      I    *
* R          R4    Dimensionless radial coordinate      -      I    *
* R0         R4    Radius root                          cm     I    *
* HSC        R4    Root length                         cm     I    *
* R1         R4    Radius soil cylinder                 cm     I    *
* T          R4    Time in scaled units                 day/cm2 I    *
* TIME       R4    Time in absolute units               day     I    *
* DELT       R4    Time step in scaled units            day/cm2 I    *
* WC         R4    Water content                       -      I    *
* WCN        R4    New values of water content          -      I    *
* DWCDT      R4    Rate of change of water content      cm2/day I    *
* BAL        R4    Balance of water in soil             cm     I    *
* RUPW       R4    Rate of uptake of water              cm/day I    *
* CUPW       R4    Cumulative water uptake              cm     I    *
* RUPWSR     R4    As RUPW and CUPW but calculated with cm/day I    *
* CUPWSR     R4    steady-rate approximation           cm     I    *
* WCAV       R4    Average water content                -      I    *
* WCAPP      R4    Average water content calculated by steady- -      I    *
*                  rate approximation                  *
*                                                     *
* Subroutines called: none                           *
*                                                     *
* Functions called:                                   *
*   FLPL: calculates matric flux potential as a function of *
*         water content                                  *
*                                                     *
* File usage:                                         *
*   detailed output written to unit 41, soilname.PET  *
*   Plot-output written to soilname.PLO              *
*-----*

```

```

SUBROUTINE OUTP(IR,R,R0,HSC,R1,T,TIME,DELT,WCN,WC,DWCDT,DIFD,
1          BAL,RUPW,RUPWSR,CUPW,CUPWSR,WCAV,WCAPP)

```

```

DIMENSION WCN(30),WC(30),DWCDT(30),DIFD(30)
DIMENSION USTR(30),WCSTR(30),U(30),R(30)
REAL KS,M,N,L

```

```

RHO=R1/R0
ETA=HSC/R0

```

```

*-----* U(I) matric flux potential
DO 5 I=1,IR
5  U(I)=FLPL(WC(I))

```

```

      USUM=0.
      DO 10 K=1,IR-1
        USUM=USUM+
1      (R(K+1)-R(K))*(R(K+1)*U(K+1)+R(K)*U(K))/2.
10    CONTINUE
      QT=RHO**2/(2.*ETA)*RUPW*RO

      UAVAPP=FLPL(WCAPP)
      USUM=2.*HSC*RO**2*USUM/R1**2
      UAV=USUM*R1**2/(HSC*(R1**2-RO**2))
      USTR(1)=FLPL(WC(1))

*----- USTR(I) matric flux potential calculated with
*----- steady-rate approximation
      DO 20 K=2,IR
        USTR(K)=USTR(1)+QT*
1      ((R(K)**2-1.)/(2.*(RHO**2-1.)))-
2      RHO**2*ALOG(R(K))/(RHO**2-1.))
20    CONTINUE

      IF(TIME.EQ.0.)THEN
        WRITE(48,100)
      ENDIF

      WRITE(41,101) T,TIME,DELT,BAL,WCAV,WCAPP
      PRINT 101,T,TIME,DELT,SUMW,BAL,WCAV,WCAPP
      WRITE(41,102) (R(K),WC(K),DWCDT(K),WCN(K),
1      DIFD(K),K=1,IR)
      WRITE(41,103) (R(K),U(K),USTR(K),K=1,IR)
      WRITE(41,*)
      WRITE(41,*) 'UAV = ',UAV,' UAVAPP = ',UAVAPP
      WRITE (41,*) 'CUPW = ',CUPW,' CUPWSR = ',CUPWSR
      WRITE(48,104) TIME,RUPW,RUPWSR,CUPW,CUPWSR
      RETURN

100  FORMAT(1X,11X,'TIME',10X,'RUPW',10X,'RUPWSR',5X,'CUPW',
1      4X,'CUPWSR')
101  FORMAT(/10X,'T='1PE15.5,2X,'REAL TIME='1PE15.5,
1      1X,'DELT='1PE15.5/
2      1X,'BAL='1PE15.5,
3      /1X,'WCAV ='1PE15.5,1X,'WCAPP ='1PE15.5)
102  FORMAT(/
1      1X,14X,'R',13X,'WC',10X,'DWCDT',12X,'WCN'
2      ,11X,'DIFD'/
3      (1X,1P5E15.5))
103  FORMAT(/1X,14X,'R',14X,'U',11X,'USTR'/
1      (1X,1P3E15.5))
104  FORMAT(1X,1P3E15.5,2F10.2)
      END

```

Appendix III. Calculation of uptake of a nutrient by a root system.

This calculation is performed by the subroutine UPTA. As input it needs the average root radius, the nitrogen demand of the crop, and the distribution with depth of root length density, water content, water uptake, concentration of the nutrient.

In the DO-loop 10 the potential uptake PUPT in mg/(cm³ soil. day), i.e. uptake in the zero-sink situation, is calculated. It is calculated from (7) as:

$$\pi L_{rv} D \frac{(\rho^2 - 1)}{G(\rho, \nu)} \tau ,$$

where L_{rv} is the root length density in cm/cm³.

Prior to the actual iteration FLAG(I), a marker which indicates if uptake from a layer can proceed as required, is in DO-loop 15 set equal to 0, for all I. The uptake from each soil layer, as described in the main text section 3.1, is performed in the DO-loop 30. The DO 30 starts with calculation of the required uptake per cm root.

In the DO 40, nested within DO 30, the actual uptake is set equal to the required uptake, if the latter is less than the potential uptake, if not actual uptake is set equal to potential uptake and FLAG for this layer is set equal to 1. Next it is investigated if the uptake does not exceed a maximum value imposed upon it by on the one hand the amount present in the layer, on the other hand the maximum flux over the root. Finally the N-requirement is updated by subtracting from it the calculated uptake if FLAG = 1, because in that case the roots take up at maximum rate. Also the total root length is updated by subtracting the root length in the layer if FLAG = 1.

In the last part of DO 30 it is investigated if the iteration can be ended, either because total uptake rate equals N-demand, or all roots take up at maximum rate.

```

*-----*
* Subroutine UPTA                                     *
* Purpose: calculation uptake of linearly adsorbed nutrient by a root *
*          system. Roots are uniformly distributed within a layer, but *
*          vertically root distribution is non-uniform.                *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time)      *
* name   type meaning                                     units   class *
*-----*-----*-----*-----*-----*
* RO     R4   radius of the root                          cm       I   *
* LRV    R4   Root density                                cm/cm3    I   *
* DIF    R4   diffusion coefficient                        cm2/day   I   *
* WCACT  R4   water content                                ml/cm3    I   *
* THCKN  R4   thickness layers                            cm        I   *
* IN     R4   number of rooted layers                     -         I   *
* CONC   R4   concentration of nutrient in soil solution  mg/ml     I   *
* TRR    R4   water uptake by the roots from a layer      cm/day    I   *
* NDEM   R4   nitrogen demand                            kg/(ha.day) I   *
* NUPTR  R4   realized total uptake rate                  kg/(ha.day) 0   *
* FMAX   R4   maximum flux through root surface          day       T   *
* DELT   R4   timestep                                    day       T   *
* NUPTR  R4   realized total uptake rate                  kg/(ha.day) 0   *
* UP     R4   Uptake from soil layer                      mg/(cm3.day) 0   *
*                                     or kg/(ha.day)         *
* PUP    R4   potential uptake from soil layer            kg/(ha.day) 0   *
*-----*
* Functions called:                                     *
*   GRNU: calculates G-function                         *
*-----*

```

```

SUBROUTINE UPTA(RO,LRV,DIF,
1   WCACT,THCKN,IN,CONC,
2   TRR,NDEM,FMAX,DELT,NUPTR,UP,PUP)

```

```

IMPLICIT REAL (A-H,J-Z)
IMPLICIT INTEGER (I)
DIMENSION WCACT(10),THCKN(10),TRR(10),NCON(10)
DIMENSION NU(10),LRV(10),DIF(10), SAMPD(10)
DIMENSION BUF(10),CONC(10),FLAG(10),UP(10)
DIMENSION MXUPT(10),G(10),RHO(10),PUP(10),PUPT(10)

```

```

*----- Specific surface root (root surface per unit root length)
PI=4.*ATAN(1.)
SPSUR=2.*PI*RO

```

```

*----- Calculation of total root length in cm/(cm2 soil surface)
TOTRL=0.
DO 5 I=1,IN
    TOTRL=TOTRL+LRV(I)*THCKN(I)
5   CONTINUE
TOTRU=TOTRL

```

```

*----- Calculation dimensionless massflow (NU), radius soil cylinder (RHO),
*          potential uptake PUPT
      DO 10 I=1,IN
        NU(I)=TRR(I)*0.5/(2.*PI*THCKN(I)*DIF(I)*LRV(I))
        RDE=LRV(I)
        RHO(I)=1./(RO*SQRT(PI*RDE))
        TNU=2.*NU(I)
        G(I)=GRNU(TNU,RHO(I))
        PUPT(I)=LRV(I)*PI*(RHO(I)**2-1.)*CONC(I)/G(I)*DIF(I)
10    CONTINUE

*----- Putting iteration flag to zero
      DO 15 I=1,IN
        FLAG(I)=0.
15    CONTINUE

      IF(TOTRU.EQ.0.)GO TO 20
*----- NREQ required uptake in mg/(cm2.day)
      NREQ=NDEM/100.
      TUP=0.
      DO 30 IJK=1,100
*----- RUPTM required uptake per cm root mg/(cm.day)
        RUPTM=NREQ/TOTRU
        DO 40 I=1,IN
          IF(FLAG(I).GT.0.)GO TO 40
          IF(PUPT(I).GT.(LRV(I)*RUPTM))THEN
            UP(I)=RUPTM*LRV(I)
          ELSE
            UP(I)=PUPT(I)
            FLAG(I)=1.
          ENDIF
        ENDIF

*----- MXUPT is least upper bound on uptake , maximum uptake
*----- is bounded by the amount of nutrient present, and the
*----- maximum flux through the root surface.
        MXUPT(I)=AMIN1(WCACT(I)*CONC(I)/DELT,FMAX*LRV(I)
1          *SPSUR)
        IF(UP(I).GT.MXUPT(I))THEN
          UP(I)=MXUPT(I)
          FLAG(I)=1.
        ENDIF

        IF(CONC(I).LE.0.)THEN
          UP(I)=0.
          FLAG(I)=1.
        ENDIF

*----- Remaining part of N-demand and total root length
*----- are calculated
        NREQ=NREQ-THCKN(I)*UP(I)*FLAG(I)
        TOTRU=TOTRU-LRV(I)*THCKN(I)*FLAG(I)
40    CONTINUE

```

```

      TUP=0.
      DO 45 I=1,IN
        TUP=TUP+THCKN(I)*UP(I)
45    CONTINUE
      CRIT=ABS((NDEM-100.*TUP)/NDEM)
      IF(CRIT.LE.1.E-5.OR.TOTRU.LE.1.E-4)GO TO 20
30    CONTINUE
20    CONTINUE

*----- conversion of mg/(cm3.day) to kg/(ha.day)
      NUPTR=0.
      DO 50 I=1,IN
        UP(I)=100.*THCKN(I)*UP(I)
        PUP(I)=100.*THCKN(I)*PUPT(I)
        NUPTR=NUPTR+UP(I)
50    CONTINUE
      RETURN
      END

```


APPENDIX IV. Calculation of water uptake by a root system.

The relation between the subroutines is shown in figure AIV-1. The calculation is performed by the routine TRANSP. As input it needs information about the number of (rooted) layers, their thickness and water content, the distribution with depth of root length density, the potential transpiration, the root conductivity, and the hydraulic properties of the layers. The latter include a pair of parameter values for the calculation of the matric flux potential Φ . This calculation is based on an empirical relation between Φ and water content as found by Ten Berge (1986):

$$\Phi = \frac{Ax}{x+B} \quad (\text{AIV-1})$$

where $x = 1 - \theta/\theta_{\text{sat}}$.

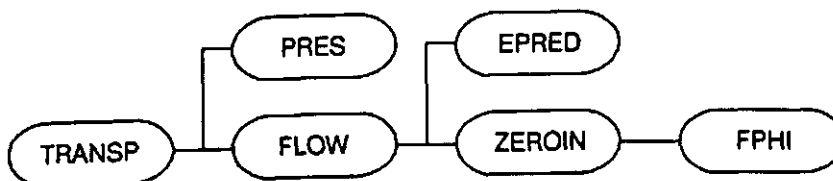
Instead of (AIV-1) of course other approximations to (8) can be used, or eventually interpolation in a table.

In TRANSP equation (15) from section 3.2 is solved for plant water potential P_p . This is done by iteration by the method of bisection during the course of which (15) written in the form:

$$H(P_p) = F_1 - E_{\text{act}} \quad (\text{AIV-2})$$

where F_1 , which stands for the left hand side of (15), has to be evaluated for different values of P_p . To do this however one must also solve the equations (14). This is achieved, again by iteration, in the subroutine FLOW, in doing so FLOW calls the function ZEROIN which finds the zero of a function in an interval. ZEROIN is given in Forsythe et al. (1977). The function EPRED calculates the actual transpiration as a function of plant water potential and potential transpiration.

Relational diagram of subroutines in TRANSP




```

REAL WC(INLAY),DX(INLAY)
REAL WCSAT(INLAY),WCR(INLAY),ALPH(INLAY),N(INLAY)
REAL A(INLAY),B(INLAY)

```

```

REAL RSS(10),RSR(10),RUPW(10),PHIMAX(10)
REAL P(10),S(10),UPW(10),R1(10),RHO(10)
REAL PHI(10),PHIRZ(10),UPRL(10),RD(10)
REAL V(10),PRZ(10),WCRZ(10),Q(10),K1,K2,LP

```

```

LOGICAL INITIAL

```

```

DATA INITIAL/.TRUE./
DATA PLIM/1.6E4/
DATA DPO/500./

```

```

*----- initialisation

```

```

IF(.NOT.INITIAL)GO TO 8
PI=4.*ATAN(1.)

```

```

DO 5 I=1,INLAY
PHIMAX(I)=A(I)/(1.+B(I))
5 CONTINUE

```

```

INITIAL=.FALSE.

```

```

8 CONTINUE

```

```

*-----

```

```

*----- calculation of root (Q(I),V(I),SV,SQ) - and soil (S(I),SS)
*----- resistance parameters, radius (R1(I)) of soil cylinder, and
*----- matric potential P(I)

```

```

K2=-K1*DPO
SV=0.
SQ=0.
SS=0.
DO 10 I=1,NRT
R1(I)=1./SQRT(PI*RD(I))
RHO(I)=R1(I)/R0
S(I)=DX(I)/R1(I)**2*(RHO(I)**2-1.)/G(RHO(I))
SS=SS+S(I)
Q(I)=RD(I)*K1*DX(I)
V(I)=RD(I)*K2*DX(I)
P(I)=PRES(WC(I),WCSAT(I),WCR(I),N(I),ALPH(I))
SV=SV+V(I)
SQ=SQ+Q(I)

```

```

10 CONTINUE

```

```

*-----

```

```

*----- first estimate of plant water potential (PP) in cm

```

```

PP=500.
DO 15 I=1,NRT
IF(PP.GT.P(I))PP=P(I)

```

```

15 CONTINUE

```

*-----

*----- two values of plant potential (PP1 resp. PP2) are
 *----- sought, for which (F1-EACT) has opposite sign

```

      PP1=1.
      PP2=1.
      DO 20 ITEL=1,20
        CALL FLOW(INLAY,EPOT,WC,P,A,B,Q,V,S,PP,N,
          $          PHIMAX,WCSAT,WCR,ALPH,
          $          PHIRZ,EACT,F1,F2,REDPOT)
        IF(EACT.EQ.0.0.AND.ABS(F1-EACT).LE.0.001)GO TO 40
        IF((F1-EACT).LT.0.)THEN
          PP1=PP
          PP=3.*PP
        ELSE
          PP2=PP
          GO TO 25
        ENDIF
      20    CONTINUE
      25    CONTINUE
  *----- done

```

*----- Now (F1-EACT)=0 is solved for PP, by method of bisection

```

      DO 30 IK =1,30
        PP=(PP1+PP2)/2.
        CALL FLOW(INLAY,EPOT,WC,P,A,B,Q,V,S,PP,N,
          $          PHIMAX,WCSAT,WCR,ALPH,
          $          PHIRZ,EACT,F1,F2,REDPOT)
        DENOM=EACT
        IF(EACT.EQ.0.)DENOM=1.
        IF(ABS(F1-EACT)/DENOM.LT..001)GO TO 40

        IF((F1-EACT).LT.0.)THEN
          PP1=PP
        ELSE
          PP2=PP
        ENDIF
      30    CONTINUE
      40    CONTINUE
  *----- done

```

```

      SQP=0.
      DO 60 IX=1,NRT
        X=1.-WC(IX)/WCSAT(IX)
        PHI(IX)=A(IX)*X/(B(IX)+X)
        WCRZ(IX)=WCSAT(IX)+PHIRZ(IX)*B(IX)*WCSAT(IX)/(PHIRZ(IX)
          1      -A(IX))
        PRZ(IX)=PRES(WCRZ(IX),WCSAT(IX),WCR(IX),N(IX),ALPH(IX))
        SQP=SQP+Q(IX)*PRZ(IX)
        UPW(IX)=(Q(IX)*(PP-PRZ(IX))+V(IX))
        UPRL(IX)=UPW(IX)/(RD(IX)*DX(IX))
        RSS(IX)=ABS(P(IX)-PRZ(IX))/(UPW(IX))

```

```

        RSR(IX)=ABS(PP-PRZ(IX))/(UPW(IX))

        IF(EACT.NE.0.)THEN
            RUPW(IX)=UPW(IX)/(EACT)
        ELSE
            RUPW(IX)=0.
        ENDIF
60      CONTINUE

        WRITE (89,*)
        WRITE (89,*)
        WRITE (89,*) 'TIME = ',DAY
        WRITE(89,100) PP,EACT,EPOT,F1
100      $ FORMAT(1H0,'PP = '1PE15.5,/1X,'EACT = '1PE15.5/1X,
        $ 'EPOT = '1PE15.5/1X,'F1 = '1PE15.5)
        WRITE(89,101) (I,WC(I),P(I),PHIRZ(I),PHI(I),UPW(I),I=1,NRT)
101      $ FORMAT(/1X,4X,'I',10X,'WC',11X,'P',8X,'PHIRZ',9X,'PHI',
        $          9X,'UPW'/
        $          (1X,I5,5E12.5))
        WRITE(89,102) (I,UPRL(I),RUPW(I),RSS(I),RSR(I),I=1,NRT)
102      $ FORMAT(/1X,4X,'I',11X,'UPRL',11X,'RUPW',12X,'RSS',12X,'RSR'/
        $          (1X,I5,4E15.5))

        END

```

```
* Subroutine FLOW
* Purpose: finds the value of the matric flux potential at the root wall,
*           for which the flow through the rhizosphere equals the flow over
*           the root wall, i. e. for each soil layer it solves:
*           Q(I)*(PP-PRZ(i))+V(I)-S(I)*(PHIRZ(I)-PHI(I)), or
*           FPHI= Q(I)*(PP-PRZ(i))+V(I)-S(I)*(PHIRZ(I)-PHI(I))-0
*
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time)
* name      type meaning                      units   class
* -----
* INLAY     I4    number of soil layers          -       I
* WC        R4    watercontent in bulk soil      ml/cm3   I
* DX        R4    thickness layers               cm       I
* EPOT      R4    Potential transpiration        cm/day   I
* A         R4    parameter from Ten Berge equation cm2/day  I
* B         R4    " " " " " "                  -       I
* P         R4    matric potential                cm       I
* S         R4    parameter expressing the local resistance to
*                 waterflow in the soil, based on steady-rate
*                 profile in matric flux potential
* Q         R4    Resistance to waterflow in the root      cm/day   I
* PP        R4    Plant water potential            cm       I
* WCR       R4    residual watercontent            ml/cm3   I
* WCSAT     R4    saturated watercontent           ml/cm3   I
* ALPH      R4    parameter from Van Genuchten equation  cm-1     I
* REDPOT    R4    indicates if reduction on potential
*                 transpiration due to plant water potential
*                 should be taken into account.
* PHIRZ     R4    matric flux potential at root surface    cm2/day  O
* EACT      R4    actual transpiration              cm/day   O
* F1        R4    total water flow over surface root system cm/day   O
* F2        R4    total water flow vrom bulk soil to roots  cm/day   O
*
* Subroutines called: none
* Functions called:
*     EPRED: calculates reduction potential transpiration
*     FPHI: evaluates the function:
*           Q(I)*(PP-PRZ(i))+V(I)-S(I)*(PHIRZ(I)-PHI(I))
*     ZEROIN : finds zero of a function in a given interval
*
* File usage: none
```

```

SUBROUTINE FLOW(INLAY,EPOT,WC,P,A,B,Q,V,S,PP,N,
$              PHIMAX,WCSAT,WCR,ALPH,
$              PHIRZ,EACT,F1,F2,REDPOT)
REAL Q(INLAY),V(INLAY),S(INLAY),ALPH(INLAY)
REAL WC(INLAY),P(INLAY),PHIRZ(INLAY)
REAL N(INLAY),PHIMAX(INLAY)
REAL WCSAT(INLAY),WCR(INLAY),A(INLAY),B(INLAY)
REAL PHI(10)

```

COMMON /PH/ AA,BB,QQ,VV,PPHI,PPP,SS,WCS,WR, FN,ALP
EXTERNAL FPHI

SQP=0.
F1=0.
F2=0.

*----- potential transpiration EPOT is corrected for plant
*----- potential effects if REDPOT>0

EACT=EPOT
IF(REDPOT.GT.0.)EACT=EPRED(PP,EPOT)

*----- for each layer the function FPHI is solved by
*----- ZEROIN to find, for given value of plant waterpotential,
*----- the matric flux potential in the rhizosphere (PHIRZ)
*----- for which FPHI = 0.
*----- FPHI = 0 implies that watertransport through the
*----- rhizosphere equals water transport over the root wall.

DO 10 IX=1,INLAY
X=1.-WC(IX)/WCSAT(IX)
PHI(IX)=A(IX)*X/(B(IX)+X)
P(IX)=PRES(WC(IX),WCSAT(IX),WCR(IX),N(IX),ALPH(IX))

*----- First two values of PHIRZ are sought for
*----- which FPHI>0, resp. <0

PHIRZ1=PHI(IX)-0.5
IF(PHIRZ1.LE.0.)THEN
PHIRZ1=.01
ELSE
ENDIF
WCRZ=WCSAT(IX)+PHIRZ1*B(IX)*WCSAT(IX)/(PHIRZ1-A(IX))
PRZ=PRES(WCRZ,WCSAT(IX),WCR(IX),N(IX),ALPH(IX))
AA=A(IX)
BB=B(IX)
QQ=Q(IX)
VV=V(IX)
PPHI=PHI(IX)
PPP=PP
SS=S(IX)
WCS=WCSAT(IX)
WR=WCR(IX)
FN=N(IX)
ALP=ALPH(IX)
FPHI1=FPHI(PHIRZ1)

PHIRZ2=PHI(IX)+0.2
IF(PHIRZ2.GE.PHIMAX(IX))THEN
PHIRZ2=PHIMAX(IX)
ENDIF
WCRZ=WCSAT(IX)+PHIRZ2*B(IX)*WCSAT(IX)/(PHIRZ2-A(IX))
PRZ=PRES(WCRZ,WCSAT(IX),WCR(IX),N(IX),ALPH(IX))

```

FPHI2=FPHI(PHIRZ2)
IF(FPHI2.GT.0.)THEN
  PHIRZ2=PHIMAX(IX)
ENDIF
FPHI2=FPHI(PHIRZ2)
IF((FPHI1*FPHI2).GT.0.)THEN
  PRINT *, 'FPHI1.2 SAME SIGN'
  PRINT *, 'PHIRZ1, PHIRZ2 ', PHIRZ1, PHIRZ2
  PRINT *, 'PHI(IX) ', PHI(IX)
  PRINT *, 'FPHI1, FPHI2 ', FPHI1, FPHI2
  PRINT *, 'PHIMAX ', PHIMAX(IX)
9  PRINT *, 'GIVE PHIRZS'
  READ *, PHIRZS
  WCRZ=WCSAT(IX)+PHIRZS*B(IX)*WCSAT(IX)/(PHIRZS-A(IX))
  PRZ=PREZ(WCRZ,WCSAT(IX),WCR(IX),N(IX),ALPH(IX))
  FPHIRS=FPHI(PHIRZS)
  PRINT *, 'FPHIRS ', FPHIRS
  PRINT *, 'ANOTHER GO? >0'
  READ *, ANGO
  IF(ANGO.GT.0.)GO TO 9
  PRINT *, 'GIVE PHIRZ1, PHIRZ2 '
  READ *, PHIRZ1, PHIRZ2
ELSE
  ENDIF
*----- Done, two values for which FPHI has
*----- opposite sign are PHIRZ1, and PHIRZ2

*----- Now FPHI=0 is solved for PHIRZ
  PHIRZ(IX)=ZEROIN(PHIRZ1, PHIRZ2, FPHI, .00001)
  FPHIRZ=FPHI(PHIRZ(IX))
  WCRZ=WCSAT(IX)+PHIRZ(IX)*B(IX)*WCSAT(IX)/(PHIRZ(IX)-A(IX))
  PRZ=PREZ(WCRZ,WCSAT(IX),WCR(IX),N(IX),ALPH(IX))

*----- F1 = Total flow over root wall
  F1=F1+Q(IX)*(PP-PRZ)+V(IX)
*----- F2 = Total flow through rhizosphere
  F2=F2+S(IX)*(PHIRZ(IX)-PHI(IX))

10  CONTINUE
    RETURN
    END

```



```

*-----*
* Function EPRED                                     *
* Purpose: calculation of actual transpiration by reduction of potential *
*           transpiration due to plant water potential PP                *
*           For PP < 5000 cm, no reduction,                             *
*           for 5000<PP<16000 reduction linearly interpolated between    *
*           (5000,1) and (16000,0.1)                                     *
* FORMAL PARAMETERS: (I=input,O=output,C=control,IN=init,T=time)        *
* name   type meaning                                     units   class *
*-----*-----*-----*-----*-----*
* PP      R4   Plant water potential                      cm       I   *
* EPOT     R4   Potential transpiration                  cm/day    I   *
* EPRED    R4   Reduced transpiration                    cm/day    0   *
*-----*

```

```

FUNCTION EPRED(PP,EPOT)
DATA P1/5000./
DATA P2/16000./

RED=1.
IF(PP.GT.P1)THEN
  RED=(0.1-1.)/(P2-P1)*(PP-P1)+1.
ELSE
ENDIF
IF(RED.LT.0.)RED=1.E-4
EPRED=RED*EPOT
RETURN
END

```

```

*-----*
* Function FPHI                                     *
* Purpose : FPHI evaluates the function:          *
*           FPHI= Q(I)*(PP-PRZ(i))+V(I)-S(I)*(PHIRZ(I)-PHI(I))          *
*           the zero of which is sought.          *
* Only input the matric flux potential at the root surface PHIRZ,      *
* other variables and parameters input via COMMON, as required by      *
* calling function ZEROIN.                                              *
*-----*

```

```

FUNCTION FPHI(PHIRZ)
COMMON /PH/ AA,BB,QQ,VV,PPhi,PPP,SS,WCS,WR,FN,ALP
WCP=WCS+PHIRZ*BB*WCS/(PHIRZ-AA)
PRZ=PRZ(WCP,WCS,WR,FN,ALP)
FPHI=QQ*PPP-QQ*PRZ+VV-SS*(PHIRZ-PPhi)
RETURN
END

```

```

FUNCTION G(R)
G=0.5*((1.-3.*R**2)/4. + R**4*ALOG(R)/(R**2-1.))
RETURN
END

```