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Verification of a mathematical model by simulating potassium uptake from soil

Verifizierung eines mathematischen Modells durch Simulation der Kaliumaufnahme aus dem Boden

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Summary This work develops the mathematical models suggested by various authors to simulate nutrient uptake of plants from soil. The simulation is based on ion transport from the soil to the roots by mass flow and diffusion and on Michaelis-Menten kinetics of nutrient uptake from soil solution by plant roots. For this purpose a differential equation is numerically integrated. Inter-root competition is allowed for by the choice of the boundary conditions. The integration procedure used makes it possible to take into account a variable buffer power which depends on soil solution concentration.

The model calculates the change of nutrient concentrations in soil as a function of distance from the root surface for preestablished periods of time. Furthermore, the rate of uptake and the quantity of nutrients taken up per cm of root length is obtained. If the growth function of the root is known, nutrient uptake of a growing root system can be calculated.

In order to verify the model two experiments were made:
1. Potassium distribution was measured in a soil in the vicinity of rape roots under three different K levels. The calculated values agreed with the measured data.
2. Potassium uptake of maize plants was measured in pot experiments with three different soils at two K levels each. Calculated K uptake agreed satisfactorily with measured K uptake.

It is therefore concluded that the theoretical conception of the model is realistic and that the parameters have correctly been measured. The model thus appears to be useful to simulate such aspects of nutrient uptake of plants from soil which cannot be measured.

Zusammenfassung Die Arbeit hat das Ziel, die von verschiedenen Autoren vorgeschlagenen Rechenmodelle zur Beschreibung der Nährstoffaufnahme aus dem Boden zu entwickeln. Sie basieren auf dem Nährstofftransport vom Boden zur Wurzel durch Massenfluss und Diffusion sowie auf der Kinetik der Nährstoffaufnahme von Wurzeln aus der Bodenlösung nach der Michaelis-Menten-Kinetik. Dabei wird eine Differentialgleichung numerisch integriert. Die Konkurrenz der Wurzeln um Mineralstoffe wird durch die Wahl der Randbedingungen berücksichtigt. Das gewählte Integrationsverfahren ermöglicht die Einbeziehung einer variablen, von der Konzentration der Bodenlösung abhängigen Pufferung.

Das Modell errechnet die Änderung der Konzentration von Mineralstoffen im Boden mit zunehmender Entfernung von der Wurzeloberfläche in beliebigen Zeitspannen. Weiterhin wird die Aufnahmerate und die Nährstoffaufnahme pro cm Wurzel ermittelt. Ist die Wachstumsfunktion der Wurzeln bekannt, so kann auch die Nährstoffaufnahme eines wachsenden Wurzelsystems errechnet werden.

Zur Verifizierung des Modells wurden zwei Versuche durchgeführt:
1. Ein Boden wurde auf drei K-Gehalte gebracht und die Verteilung der K-Konzentration in der Umgebung von Rapswurzeln gemessen. Die Modellrechnung ergab eine gute Übereinstimmung zwischen der gemessenen und der errechneten Konzentrationsverteilung im wurzelnahen Boden.
2. In einem Gefässversuch mit drei Böden und je zwei K-Stufen wurde die K-Aufnahme von Maispflanzen gemessen. Auch hier stimmte die gemessene K-Aufnahme mit dem Ergebnis der Modellrechnung befriedigend überein

Hieraus wird der Schluss gezogen, dass die theoretischen Vorstellungen, die dem Modell zugrundeliegen, realistisch sind und die verwendeten Parameter richtig gemessen wurden. Das Rechenmodell erscheint daher geeignet, um auch solche Aspekte der Mineralstoffaufnahme aus dem Boden zu untersuchen, die man nicht messen kann.

Introduction

Nutrient uptake of plants from soil is the result of interactions between plant and soil. The rate of uptake of a nutrient depends on the concentration of this nutrient in soil solution at the root surface. The relation between the concentration and the rate of uptake can often be described quantitatively by Michaelis-Menten-kinetics as has been published by Epstein[8] and Nielsen[12]. Barber[2] has shown that transport of nutrients from soil to plant roots essentially proceeds by mass flow and diffusion. The determinants of these mechanisms are also known; therefore, they can be described mathematically. By combining the uptake and transport processes in a mathematical model, it appears possible to calculate the whole process of nutrient uptake of plants from soil under the influence of the plant and soil factors involved. By comparing the results from simulation with those from experiments, it should be possible to check the correctness of our ideas about the interaction between plant and soil in regard to nutrient uptake of plants. Furthermore, the significance of the factors involved can be assessed and such parts of the whole system that cannot be measured can be calculated.

Models of this kind have been developed by several authors[4,5,6,7]. The model of Nye and Marriott[14] describes the distribution of nutrients around the root. Claassen and Barber[5] extended the model in order to determine also the rate of uptake and the quantity of a nutrient taken up per unit of roots as a function of time of uptake. Another supplement enables the calculation of total nutrient uptake of growing root systems. This gives a possibility to verify the model since the quantity of nutrients taken up can be measured easily.

Cushman[6] has changed one of the boundary conditions for integrating the differential equation in order to include the competition for nutrients among neighbouring roots. This is important for nutrients high enough in mobility to allow for an overlap of the depletion profiles of neighbouring roots.

Since Cushman[6] integrates the differential equation analytically, he has to assume a linear relationship between the uptake rate and soil solution concentration. Therefore, the application of the model is restricted to relatively low concentrations of nutrients in soil. However, this is often not so, for example in the case of potassium or nitrate.

This restriction was overcome in later developments by Barber and Cushman[4] and Cushman[7] by using numerical integration of the differential equation which allows for a nonlinear relationship between uptake rate and soil solution concentration.

This approach was used in this research, *i.e.*, nutrient uptake from soil solution is described by Michaelis-Menten kinetics and root competition is accounted for.

The aim of the present study was to test this model by comparing calculated and measured total K uptake by a growing root system under very different soil conditions, which has been done by several authors as described by Barber[3]. It furthermore should be tested by comparing the measured and calculated nutrient depletion next to root surfaces. This has not been done before and is an important step in the overall process of nutrient uptake from soil.

Description of the model

The model is based on the differential equation (1) taken from Nye and Marriott[15] which describes the transport of nutrients to the root by mass flow and diffusion.

$$\frac{dC_l}{dt} = \frac{1}{r}\frac{d}{dr}\left(r \cdot D_e \frac{dC_l}{dr} + \frac{v_0 \cdot r_0 \cdot C_l}{b}\right) \qquad (1)$$

C_l = concentration of the soil solution
r = radial distance from the root axis
r_0 = root radius
D_e = effective diffusion coefficient
b = buffer power
v_o = rate of water uptake
t = time

The integration was performed under the following initial and boundary conditions:

$$t = 0, r > r_0, C_l = C_{li} \qquad (2)$$

$$t > 0, r = r_0, De \cdot b \frac{dC_l}{dr} + v_0 C_l = \frac{I_{max}(C_l - C_{lmin})}{K_m + C_l - C_{lmin}} \qquad (3)$$

$$t > 0, r = r_1, D_e \cdot b \frac{dC_l}{dr} + \frac{r_0}{r_1} v_0 C_l = 0 \quad (4)$$

$$\text{or } C_l = C_{li}$$

In this case is

C_{li} = initial concentration of the soil solution
C_{lmin} = minimum concentration; net influx = 0
k_m = Michaelis constant
I_{max} = maximum rate of net influx
r_1 = half distance between roots

Equation (3) states that the flux of nutrients at the root surface equals the rate of uptake which in turn follows Michaelis-Menten kinetics as formulated by Nielsen[12].

Equation (4) allows for inter-root competition and indicates that between two neighbouring roots is a flux of water but not of nutrients[6]. Equation (4a) is the alternative to equation (4) for non inter-root competition *i.e.* at r_1 the concentration is kept constant and equal to C_{li}.

The solution of the problem defined by equation (1) to (4) is obtained numerically by an implicit finite-difference method. Because of the nonlinearity introduced by equation (3) the resulting system of equations is solved by the iterative Newton-Raphson[7,16] algorithm.

It shows rapid convergence and is unconditionally stable. It furthermore allows the introduction of a concentration dependent buffer power. The relation between buffer power and soil solution concentration can be of any form.

The computer program was written in 'BASIC' and executed on a Commodore computer. It calculates the rate of uptake for preestablished time steps, the cumulative quantity of nutrients (AM) taken up per cm of root, and the distribution of the nutrients around the root after each time step. Total uptake of a growing root system (GA) is then obtained from the sum of the products of root segments, L_a, (with the period of uptake 'a'). t is the duration of the uptake experiment.

$$GA = \sum_{a=0}^{a=t} \Delta L_a AM_a \quad (5)$$

In order to determine ΔL_a values, at least two harvests are necessary. By using a growth function, which may be linear or exponential the proportion of the root system of age 'a' can be calculated. For young plants as used in this research the root growth function has been found to be exponential.

Table 1. Some properties of the soils used

Soil		Clay (%)	pH	Exch. K (μmol/100 g)
1 Söderhof	K_1 *	9.2	7.2	295
2 Söderhof	K_2	9.2	7.2	517
3 Söderhof	K_3	9.2	7.2	1365
4 Bründeln	K_1	12.1	7.8	303
5 Bründeln	K_2	12.1	7.8	440
6 Bülten	K_1	21.2	8.0	132
7 Bülten	K_3	21.2	8.0	268
8 Herrenhs.	K_1	4.4	7.1	199
9 Herrenhs.	K_2	4.4	7.1	382

Tabelle 1. Eigenschaften der verwendeten Böden

* Subscripts 1 = soil was cropped to lower K content of the soil
2 = soil was untreated
3 = soil was fertilized with K

Materials and methods

Some properties of the soils used are summarized in Table 1. In order to obtain varying K contents, the soils were cropped with maize, left unchanged or fertilized with K. Potassium depletion profiles were determined with soils 1–3; soils 4–9 were used in a pot experiment in order to determine K uptake of maize plants.

Determination of K depletion profiles

K distribution in the soil adjacent to the roots was obtained from[10]. For this purpose, pregerminated seeds of oil seed rape c.v. 'Quinta' were grown in special containers in which the roots were separated from the soil by a fine meshed Nylon screen. Root hairs penetrated through the screen into the soil, but the roots could not. In this way, a plane interface between the root system and the soil was obtained. The pots were placed on a ceramic porous plate, which was connected to a 100 cm water column in order to supply water of a tension of pF 2. After a growth period of 4 days, the plants were harvested. The soil block was frozen in liquid nitrogen and divided into thin layers by using a refrigerated microtome. The soil samples obtained this way have a defined distance from the root surface. They were extracted with 1 *N* NH_4-acetate solution in order to determine exchangeable potassium. (For details see[9]).

Pot experiment

K uptake of maize plants c.v. 'Garbo' was determined in 3 different topsoils at two levels of K in a pot experiment (as shown in Table 1, No. 4–9). In addition 280 mg N and 440 mg P per pot were added as NH_4NO_3 and $CaHPO_4$. Under constant climatic conditions two plants were grown in pots filled with 5 kg of soil. Root and shoot weight, potassium content of the plants and root length were determined 10 (11 days for soil 8) and 21 days after sowing. Roots were carefully washed out of the soil and root length measured according to Newman[13].

Determination of the soil and plant parameters

I_{max}: Maximum rate of K net influx. In case of the depletion profile experiments I_{max} was derived from the treatment with the highest K level. In this treatment exchangeable K was decreased to about 200 μmol K/100 g and, as shown by desorption studies, soil solution concentration is about 20 μmol l^{-1}. At this K concentration uptake rate is 1/3 of I_{max} if K_m equals 40 μmol l^{-1}. Therefore, the measured uptake rate was multiplied by 3 to obtain I_{max}. In the pot experiment, I_{max} is the rate of K influx measured when additional K application to the soil under study did not increase the rate of K influx.

K_m: The Michaelis constant and

C_{lmin}: the minimum concentration were determined in nutrient solution by the method of Claassen and Barber[5].

r_0: Root radius in the pot experiment was calculated from root length and root fresh weight according to

$$r_0 = \sqrt{\frac{\text{root fresh weight (g)}}{\pi \cdot \text{root length (cm)}}}$$

In the depletion profile experiment, r was set to 1 cm for the calculation in order to simulate the plane soil-root interface.

v_0: Water uptake rate was calculated from the water consumption of the plants in the respective experiments. In the pot experiment, the rate of uptake was calculated by using the equation of Williams[17].

r_1: the mean half-distance between two neighbouring roots was calculated according to

$$r_1 = \sqrt{\frac{\text{soil volume (cm}^3\text{)}}{\pi \cdot \text{root length (cm)}}}$$

C_{li}: The initial concentration of the soil solution was measured in the displacement extract as suggested by Adams[1].

D_e: The effective diffusion coefficient was calculated from the formula

$$D_e = D_l \sim f \frac{1}{1}$$

D_l = diffusion coefficient in water

θ = volumetric water content of the soil

f = impedance factor, being mainly a function of θ was obtained from Fig. 4.1 out of[15]

b = buffer capacity defined as

$$\frac{\Delta C}{\Delta C_1} = \frac{C_i - C_f}{C_{li}}$$

ΔC is the decrease of exchangeable K

C_1 and C_f is the initial and final exchangeable K in a desorption experiment

k: Is the relative growth constant defined as

$$k = \frac{\ln (L_2/L_1)}{t_2 - t_1}$$

L_1 and L_2 is root length at time t_1 and t_2 when harvests one and two were made

Results

Shoot dry weight, root length, and K content of the maize plants of the pot experiment are summarized in Table 2. As can be seen, K concentrations and K uptake of the plants were markedly increased by the application of K to the soils. These data were used to test the simulation model. The parameters necessary for the calculation are given in Table 3. The quantity of K taken up between the first and the second harvest was calculated according to the scheme shown in Table 4. This table indicates that 40% of the K taken up was absorbed by the roots already present at the first harvest, the other 60% was

Table 2. Root length, shoot weight and potassium content of maize plants in a pot experiment at two harvests

Soil	K level*	1. harvest Root length (cm)	1. harvest Shoot weight (g)	1. harvest K (%)	2. harvest Root length (cm)	2. harvest Shoot weight (g)	2. harvest K (%)
Bründeln	K_1	1349	0.13	1.96	7899	1.49	2.17
Bründeln	K_2	1601	0.14	2.34	12701	1.58	4.09
Bülten	K_1	1373	0.15	1.63	14201	1.60	1.88
Bülten	K_3	1009	0.11	2.42	11256	1.33	4.30
Herrenhausen	K_1	284	0.07	1.92	1922	0.53	2.76
Herrenhausen	K_2	2225	0.18	5.59	9690	2.23	5.59

Tabelle 2. Wurzellänge, Sprossertrag und K-Gehalt von Maispflanzen zur 1. und 2. Ernte im Gefässversuch

* Subscripts 1 = soil was cropped to lower K content of the soil
2 = soil was untreated
3 = soil was fertilized with K

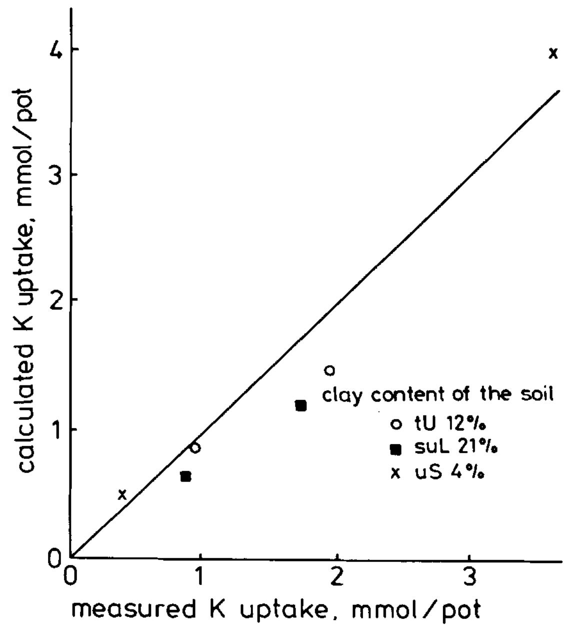

Fig. 1. Measured and calculated K uptake of maize plants in a pot experiment.

Abb. 1. Vergleich der gemessenen und errechneten K-Aufnahme von Maispflanzen in einem Gefässversuch.

Table 3. Soil and plant parameters used in the simulation model. Plants used were oil seed rape for 1, 2 and 3 and maize for the remaining soils

	Soil								
	1	2	3	4	5	6	7	8	9
Plant parameters									
I_{max}*, μmol cm^{-2} s^{-1} 10^{-6}	100	100	100	5.4	5.4	4.8	4.8	9.8	9.8
K_m, μmol cm^{-3} 10^{-2}	4	4	4	3.9	3.9	3.9	3.9	3.9	3.9
C_{lmin}, μmol cm^{-3} 10^{-3}	2	2	2	2	2	2	2	2	2
r_0*, cm 10^{-2}	100	100	100	1.70	1.38	1.42	1.55	1.73	1.64
v_0*, cm 10^{-7}	16.8	16.8	16.8	6.61	6.61	3.71	3.71	4.85	4.85
r_1*, cm 10^{-2}	280	280	280	39.4	31.0	29.4	33.0	74.3	33.1
k, s^{-1} 10^{-6}				1.7	1.8	2.1	2.3	2.0	1.5
L_1, cm				1349	1601	1373	1009	284	2225
Soil parameters									
C_{li}, μmol cm^{-3}	0.112	0.620	5.44	0.116	0.266	0.087	0.260	0.765	1.504
D_e, cm^2 s^{-1} 10^{-7}	1.10	2.21	5.64	0.72	0.99	1.33	1.66	3.09	2.90
b	14.6	7.3	2.9	22.8	16.6	12.3	9.9	2.9	3.1

Tabelle 3. Boden- und Pflanzenparameter, die zur Modellrechnung verwendet wurden, Raps für Boden 1, 2 und 3 und Mais für Boden 4 bis 9

* These parameters differ greatly for soils 1, 2 and 3 because of planar conditions of the uptake surface. Due to a large root hair density I_{max} is increased strongly. To simulate planar conditions r_0 was taken equal 1 cm and r_1 is the root radius plus the depth of the soil block.

v_0: due to the experimental set up very much larger than for single roots in soil.

Table 4. Basic data for the calculation of K uptake by a whole root system (Soil 4)

(1) t_i (d)	(2) ΔL_i (cm)	(3) age (d)	(4) AM/cm (µmol/cm)	(5) AM_i (µmol)
0	1349	11.00	0.2558	345.1
0.5	104	10.75	0.2275	23.8
1.5	234	10	0.2181	51.1
2.5	272	9	0.1990	54.2
3.5	316	8	0.1790	56.6
4.5	367	7	0.1587	58.2
5.5	426	6	0.1384	59.0
6.5	494	5	0.1173	58.0
7.5	575	4	0.0962	55.3
8.5	667	3	0.0741	49.4
9.5	774	2	0.0511	39.6
10.5	899	1	0.0270	24.3
11.0	503	0.25	0.0075	3.8
				Σ 878.4

Tabelle 4. Grunddaten zur Berechnung der K-Aufnahme eines gesamten Wurzelsystems (Boden 4).

(1) t_i = time from first harvest in days
(2) ΔL_i = $L_i - L_{i-1}$, new root growth between t_{i-1} and t_i or roots already present at $t_i = 0$
L_i = $L_1 e^{kt_i}$, L_1 = root length at first harvest and k = relative growth constant in $days^{-1}$
(3) d = age of root segment ΔL_i in days, given by $(t_2 - t_1) - (t_i + t_{i-1})/2$
(4) AM/cm = K uptake per cm after time of uptake equals the age of the root segment calculated by the model
(5) AM_i = K taken up by root segment ΔL_i equals (2) × (4).

taken up by the roots grown between the first and the second harvest.

For each of the 6 treatments the relation between calculated and measured K uptake is shown in Figure 1. This indicates that the model gave a satisfactory prediction of the K uptake of corn plants measured in this experiment.

The distribution of the K concentration in the soil around the roots of oil seed rape plants is shown in Figure 2. The fully drawn curves are the result of the simulation calculation and are not simply regression lines. It can be stated that these calculated lines are well in agreement with the measured data.

Discussion

The results have shown that the simulation model satisfactorily predicted the potassium uptake of root systems growing in soil. This confirms former results of Claassen and Barber[5]. In addition, it became apparent that the model also described adequately the distribution

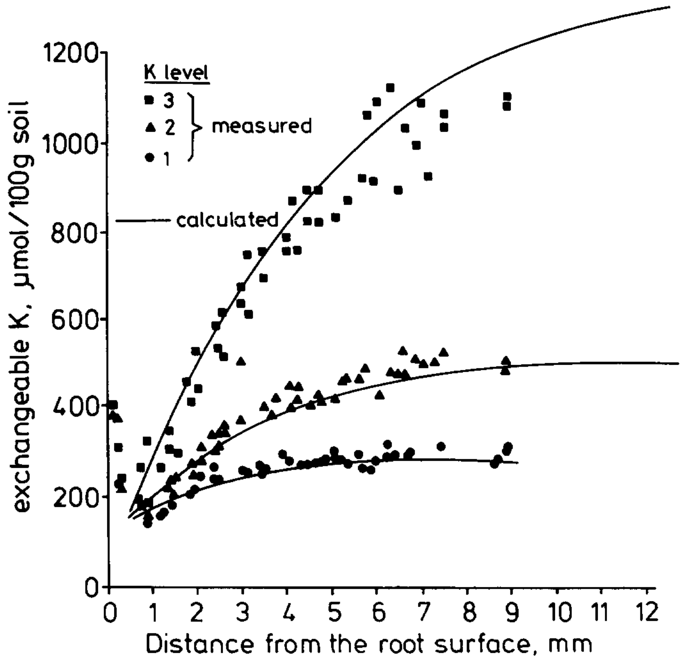

Fig. 2. Measured and calculated K concentration of the soil in the vicinity of rape roots (4 days old) at three different K levels.

Abb. 2. Vergleich der gemessenen und errechneten K-Verarmungsprofile von 4 Tage alten Rapspflanzen bei 3 verschiedenen K-Gehalten eines Bodens.

of the K concentration in the soil around the roots. The model therefore proved to be useful to simulate the whole process as well as an important aspect of the total sequence of interactions between plant roots and the soil in potassium uptake.

The model consists of two distinct parts, *i.e.*, the transport to the root by mass flow and diffusion and the uptake following Michaelis Menten kinetics. In order to test both parts the K supply of the soil should be such that transport to the plant is limiting K uptake; otherwise, because of the second boundary condition, we would only test whether I_{max} was measured correctly. For this reason, in the pot experiment, only those treatments were chosen where the K content of maize plants was below its maximum value; thereby assuring that also the transport of K through the soil had to be simulated by the model correctly.

It can thus be concluded that the model is based on a realistic conception of nutrient uptake from soil and that the parameters have been measured with sufficient accuracy. This is an encouragement to use the model also for such aspects of the soil-root interactions which cannot be measured so far; as, for example, the distribution of potassium around individual roots under different moisture levels[11].

The numerical integration of the differential equation with the Newton-Raphson method made it possible to introduce a nonlinear relationship between concentration and uptake rate as, in this case, the Michaelis-Menten equation. Therefore, the model can be applied to conditions of relatively high concentrations in the soil solution.

A copy of the computer program can be sent by the authors on request.

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