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MATHEMATICAL ANALYSIS OF DIFFUSION AND MASS FLOW OF SOLUTES TO A ROOT ASSUMING CONSTANT UPTAKE

door

P. DE WILLIGEN

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Instituut voor Bodemvruchtbaarheid, Oosterweg 92,
Postbus 30003, 9750 RA, Haren (Gr.)

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1. INTRODUCTION

Traditionally, most studies on transport of solutes in soil to a root, considered root uptake to be a function of concentration (Nye and Tinker, 1977). As is discussed elsewhere (Van Noordwijk *et al.*, in preparation) it is also possible and justifiable to assume that uptake is determined by crop demand as long as the concentration in the immediate vicinity of the root exceeds a certain limiting value. This demand is virtually constant in time for closed green canopies growing under optimum conditions. The goal of this paper is to present some analytical solutions, when such a constant uptake determines the boundary condition at the root surface. Transport by both diffusion and mass flow is considered, together with adsorption (and desorption) proceeding at a finite or infinite rate.

2. MATHEMATICAL FORMULATION

Consider a uniformly distributed root system consisting of vertical roots, with root density W cm cm^{-3}, and suppose all roots have the same length h cm and radius R_0 cm (fig. 1). To each root thus a cylinder of soil can be assigned of height h and radius R_1, the latter given by:

$$R_1 = \frac{1}{\sqrt{\pi W}} \quad \text{cm} \tag{1}$$

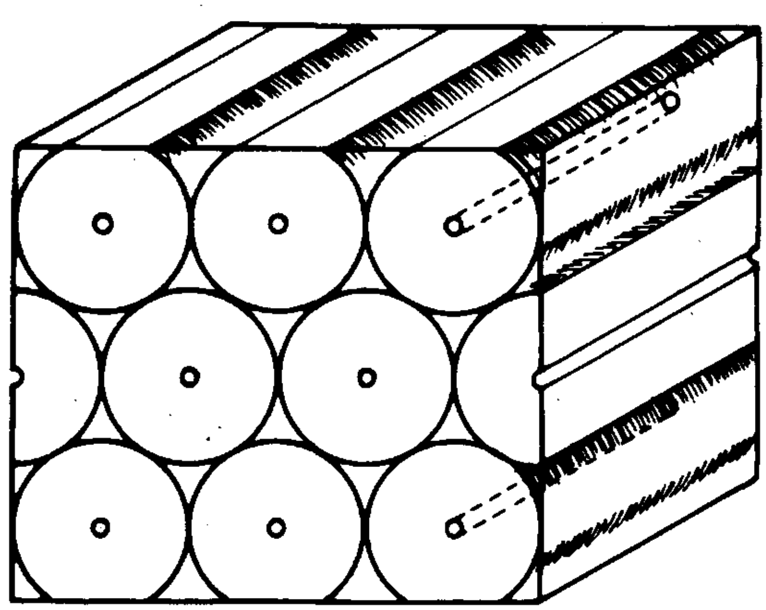

Fig. 1. Schematic representation of roots as regularly distributed, parallel axes. Root density (length of roots per volume of soil) may also be represented by the number of intersections per surface area (perpendicular to root axis). In the model the soil between the cylinders is considered to be spread out as an outer layer of each cylinder.

If transpiration amounts to E ml/(cm^{2}day) and a steady-state situation exists with respect to radial movement of water, the rate of water transport in the soil cylinder at any distance r from the root midpoint ($R_0 \leqslant r \leqslant R_1$) is E/W ml day^{-1}. So the flux of water at distance r is given by:

$$v = \frac{-E}{2\pi hrW} \text{ cm day}^{-1} \tag{2}$$

The negative sign in (2) indicates that the direction of the flux is in the negative direction of r.
Neglecting tangential and vertical gradients, the flux of solute at distance r can be given as:

$$F = -D\frac{\delta C}{\delta r} + vC$$

with

D =	combined diffusion-dispersion coefficient	$cm^2 day^{-1}$
C =	concentration of the solute in the soil solution	$mg\ ml^{-1}$
r =	radial distance from the root midpoint	cm

The equation of continuity in cylindrical coordinates is given by (Nye and Tinker, 1977):

$$\frac{\delta C_T}{\delta t} = -\frac{1}{r}\frac{\delta}{\delta r} rF$$

with

C_T =	the bulk density of solute	$mg\ cm^{-3}$
t =	time	day

When the soil is not too dry (pF < 3.5) the diffusivity usually is so high, that if root-density is not too low ($W \geqslant 0.5$), small gradients in water content suffice to transport water to the root at the required rate (Greacen, 1977). Hence the water-content will be taken constant in the following.
Substitution of the expression for the flux into the equation of continuity then yields:

$$\frac{\delta C_T}{\delta t} = \frac{D}{r}\frac{\delta}{\delta r} r\frac{\delta C}{\delta r} - v\frac{\delta C}{\delta r} \tag{3}$$

The bulk density C_T consists of two components:

$$C_T = C_A + \Theta C \tag{4}$$

where C_A = the bulk density of adsorbed solute mg cm^{-3}
Θ = the water content ml cm^{-3}

Equation (4) substituted in (3) leads to:

$$\frac{\delta C_A}{\delta t} + \Theta\frac{\delta C}{\delta t} = \frac{D}{r}\frac{\delta}{\delta r}r\frac{\delta C}{\delta r} - v\frac{\delta C}{\delta r} \tag{5}$$

If, as is assumed here, the adsorption isotherm is linear, adsorption is reversible, and proceeds according to a first order reaction, the following equation holds:

$$\frac{\delta C_A}{\delta t} = k(KC - C_A) \tag{6}$$

with
k = adsorption rate constant day^{-1}
K = adsorption coefficient ml cm^{-3}

Equations (5) and (6) constitute the system of partial differential equations, the solution of which is sought.
To complete the system, initial and boundary conditions have to be defined in conjunction with the partial differential equations. For the root system described earlier the appropriate condition at the outer boundary of the soil cylinder states the absence of transport across this boundary:

$$r = R_1 \ : \ -2\pi h R_1 D\frac{\delta C}{\delta r} + 2\pi h R_1 vC = 0 \tag{7}$$

As is implied in the title of this report and was briefly discussed in the Introduction, the condition at the root surface was chosen to reflect constant plant demand. If this demand amounts to A mg $cm^{-2}day^{-1}$, then each root has to take up A/W mg day^{-1} in order to satisfy the demand. The second boundary condition accordingly can be formulated as:

$$r = R_0 \; : \; -2\pi h R_0 D\frac{\delta C}{\delta r} + 2\pi h R_0 vC = -A/W \qquad (8)$$

In connection with the formulation of the boundary condition at the root surface a few things have to be said about the limiting concentration. This limiting concentration is a function of root-density and the relation between concentration and potential uptake. The latter usually can be represented as a Michaelis-Menten curve, which for our purposes can be thought to be composed of two straight lines (fig. 2), one parallel to the concentration axis, and the other through the origin, the slope of which is the root absorbing power (Nye and Tinker, 1977).

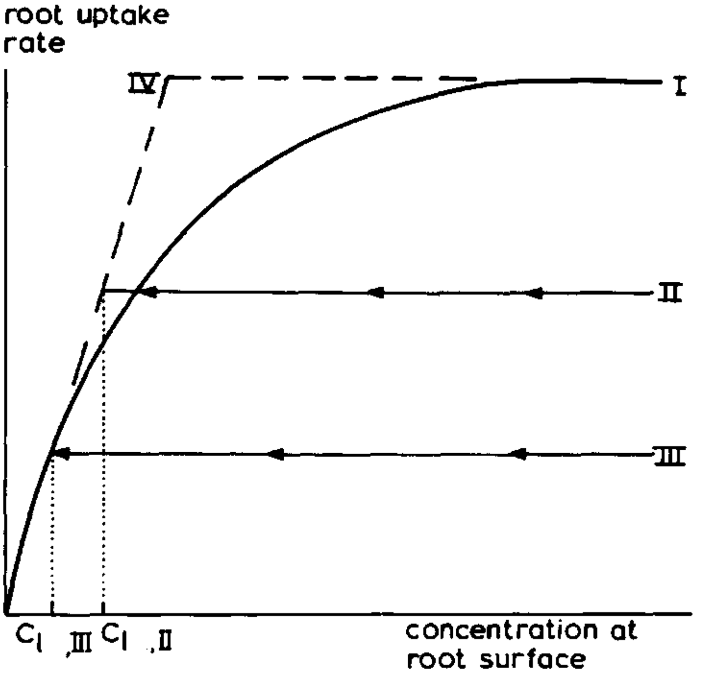

Fig. 2. Absorption per unit root as a function of the concentration at the root surface (C_{R0}). Line I represents the Michaelis-Menten relation found in short-term fysiological experiments. Line II shows that in our model absorption is taken to be independent of concentration as long as possible. In the case of line III the root density is twice as high and so the adsorption rate per root may be half the value of line II. This lower absorption rate may be sustained till a lower concentration C_1 is reached. In the calculations the broken line IV was used as the boundary instead of line I.

The limiting concentrationis that concentration, when potential uptake equals plant demand, or

$$2\pi R_0 h m C_1 = \pi R_1^2 A$$

so that C_1 can be found as:

$$C_1 = \frac{R_1^2 A}{2R_0 hm}$$

where m = root absorbing power cm day^{-1}
Initially the soil around the root is assumed to have a uniform solute bulk density, with equilibrium between adsorbed and solved solute:

$$t = 0 : C = C_i \quad C_A = C_{A_i} = K.C_i \tag{9}$$

To facilitate notation and to show the interrelation between the various variables and parameters the following dimensionless quantities were defined:

dimensionless	time	$\tau = Dt/R_0{}^2$
"	concentration	$U = C/C_i$
"	bulk density of adsorbed solute	$V = C_A/C_{A_i} = C_A/KC_i$
"	distance	$x = r/R_0$
"	flow of water	$2\nu = rv/D = -E/(2\pi hDW)$
"	root length	$\eta = h/R_0$
"	radius of soil cylinder	$\rho = R_1/R_0$
"	supply/demand parameter	$\phi = DC_i/AR_0$
"	rate constant	$\lambda = kR_0{}^2/D$
"	buffer capacity	$B = (K+\Theta)/\Theta$
"	bulk density of solute	$T = (KV+\Theta U)/\Theta B$

Note that $2\nu = \frac{-\rho^2}{2\eta\phi_w}$, where $\phi_w = D/ER_0$

Then the equations (5) and (6) and the conditions (7), (8) and (9) transform into:

$$K\frac{\delta V}{\delta \tau} + \Theta\frac{\delta U}{\delta \tau} = \frac{\delta^2 U}{\delta x^2} + \left(\frac{1-2\nu}{x}\right) \frac{\delta U}{\delta x} \tag{10}$$

$$\frac{\delta V}{\delta \tau} = \lambda(U-V) \tag{11}$$

$$x = \rho: \; -\frac{\delta U}{\delta x} + \frac{2\nu}{\rho}U = 0 \tag{12}$$

$$x = 1: \; -\frac{\delta U}{\delta x} + 2\nu U = \frac{-\rho^2}{2\eta\phi} = Q \tag{13}$$

$$\tau = 0 \quad U = V = 1 \tag{14}$$

The solution of the above system (10-14) is given by (see Appendix I for the derivation):

$$U = \left\{\frac{\rho^2-1}{\rho^{2\nu+2}-1}\right\}(\nu+1)x^{2\nu} \qquad + \tag{15a}$$

$$Q\left[\frac{2(\nu+1)x^{2\nu}}{\rho^{2\nu+2}-1}\;\frac{\tau}{\Theta B} + \frac{x^{2\nu}(x^2-\rho^2)}{2(\rho^{2\nu+2}-1)} + \frac{\rho^2(\rho^{2\nu}-x^{2\nu})}{2\nu(\rho^{2\nu+2}-1)} + \frac{\rho^2(\rho^{2\nu}-1)(\nu+1)x^{2\nu}}{2\nu(\rho^{2\nu}-1)^2} + \right.$$

$$\left. + \frac{x^{2\nu}(\nu+1)(1-\rho^{2\nu+4})}{(2\nu+4)(\rho^{2\nu+2}-1)^2} + \frac{2(\nu+1)x^{2\nu}(B-1)(1-e^{-B\lambda\tau})}{(\rho^{2\nu+2}-1)\Theta B^2\lambda}\right] + \tag{15b}$$

$$+ (Q-2\nu)x^{\nu}\pi \sum_{n=1}^{\infty} 2F_{\nu}(x, \alpha_n)\; G(s_{n_1}, s_{n_2}, \tau) \qquad + \tag{15c}$$

$$+ \frac{2\nu x^{\nu}}{\rho^{\nu+1}}\pi \sum_{n=1}^{\infty} \frac{2J_{\nu+1}(\alpha)}{J_{\nu+1}(\rho\alpha)} F_{\nu}(x, \alpha_n)\, G(s_{n_1}, s_{n_2}, \tau) \tag{15d}$$

with

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

$$s_{n_1}, {}_{n_2} = \frac{-(B\lambda\Theta+\alpha^2{}_n) \pm \sqrt{(B\lambda\Theta+\alpha^2{}_n)^2 - 4\lambda\alpha^2{}_n}}{2\Theta}$$

$$G(s_{n_1}, s_{n_2}, \tau) = \frac{e^{s_{n_1}\tau}(s_{n_1}+\lambda)^2}{s_{n_1}\Theta\{(s_{n_1}+\lambda)^2 + (B-1)\lambda^2\}} + \frac{e^{s_{n_2}\tau}(s_{n_2}+\lambda)^2}{s_{n_2}\Theta\{(s_{n_2}+\lambda)^2 + (B-1)\lambda^2\}}$$

and α_n is the n-th root of:

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

J_ν, Y_ν are Besselfunctions of first and second kind , respectively, and order ν.

The bulk density of adsorbed solute is given by:

$$V = \left(\frac{\rho^2-1}{\rho^{2\nu+2}-1}\right)(\nu+1)x^{2\nu}(1-e^{-\lambda\tau}) + \frac{2Q(\nu+1)x^{2\nu}}{(\rho^{2\nu+2}-1)}\frac{\tau}{\Theta B} +$$

$$+ Q(1-e^{-\lambda\tau})\left[\frac{-2(\nu+1)x^{2\nu}}{(\rho^{2\nu+2}-1)\lambda} + \frac{x^{2\nu}(x^2-\rho^2)}{2(\rho^{2\nu+2}-1)} + \frac{\rho^2(\rho^{2\nu}-x^{2\nu})}{2\nu(\rho^{2\nu+2}-1)} +\right.$$

$$\left. + \frac{\rho^2(\rho^{2\nu}-1)(\nu+1)x^{2\nu}}{2\nu(\rho^{2\nu}-1)^2} + \frac{x^{2\nu}(\nu+1)(1-\rho^{2\nu+n})}{(2\nu+4)(\rho^{2\nu+2}-1)^2}\right] +$$

$$+ \frac{2Q(\nu+1)x^{2\nu}(B-1)}{(\rho^{2\nu+2}-1)\Theta B^2\lambda}\left[1 - \frac{e^{-B\lambda\tau}}{1-B} + \frac{Be^{-\lambda\tau}}{1-B}\right] + e^{-\lambda\tau}$$

$$+ (Q-2\nu)x^{\nu}\pi \sum_{n=}^{\infty} 2F(x,\alpha_n)\,H(s_n, s_{n_2}, \tau)$$

$$+ \frac{2x^{\nu}}{\rho^{\nu+1}}\pi \sum_{n=}^{\infty} \frac{2J_{\nu+1}(\alpha)}{J_{\nu+1}(\rho\alpha)} F_\nu(x,\alpha_n)H(s_{n_1}, s_{n_2}, \tau) \qquad (16)$$

with

$$H(s_{n_1}, s_{n_2}, \tau) \quad \frac{(e^{s_{n_1}\tau} - e^{-\lambda\tau})(s_{n_1}+\lambda)^2}{s_{n_1}\Theta\{(s_{n_1}+\lambda)^2 + (B-1)\lambda^2\}} + \frac{(e^{s_{n_2}\tau} - e^{-\lambda\tau})(s_{n_2}+\lambda)^2}{s_{n_2}\Theta\{s_{n_2}+\lambda)^2 + (B-1)\lambda^2\}}$$

As is shown in Appendix I other solutions can be derived from (15) or (16). When transport is by diffusion only:

$$U = \quad 1 \qquad + \tag{17a}$$

$$Q\{\frac{2}{\rho^2-1}\frac{\tau}{\Theta B} + \frac{x^2-\rho^2}{2(\rho^2-1)} + \frac{\rho^2}{\rho^2-1}\ln(\frac{\rho}{x}) + \frac{\rho^2}{(\rho^2-1)^2}\ln\rho - \frac{(1+\rho^2)}{4(\rho^2-1)}$$

$$+ \frac{2}{\rho^2-1}\ \frac{(B-1)(1-e^{-B\lambda\tau})}{\Theta B^2\lambda}\} \tag{17b}$$

$$+ Q\pi \sum_{n=1}^{\infty} F_o(x,\alpha_n)G(s_{n_1},s_{n_2},\tau) \tag{17c}$$

where α_n now is the n-th root of:

$$Y_1(\rho x)J_1(x)-Y_1(x)J_1(\rho x) = 0$$

$$V = 1 + \frac{2Q}{(\rho^2-1)}\frac{\tau}{\Theta B} +$$

$$Q(1-e^{-\lambda\tau})\{\frac{-2}{(\rho^2-1)\lambda} + \frac{x^2-\rho^2}{2(\rho^2-1)} + \frac{\rho^2}{\rho^2-1}\ln(\frac{\rho}{x}) + \frac{\rho^2}{(\rho^2-1)^2}\ln\rho - \frac{(1+\rho^2)}{4(\rho^2-1}\}$$

$$+ \frac{2\ Q(B-1)}{(\rho^2-1)\Theta B^2\lambda}\{1-\frac{e^{-B\lambda\tau}}{(1-B)} + \frac{Be^{-\lambda\tau}}{(1-B)} + \frac{Be^{-\lambda\tau}}{(1-B)}\} +$$

$$+ Q\pi \sum_{n=1}^{\infty} F_o(x,\alpha_n)H(s_{n_1},s_{n_2},\tau) \tag{18}$$

The solution when adsorption is u instanteneous is given by:

$$U = (\frac{\rho^2-1}{\rho^{2\nu+2}-1})\ (\nu+1)x^{2\nu} \tag{19a}$$

$$+ Q\left[\frac{2(\nu+1)x^{2\nu}}{\rho^{2\nu+2}-1}\ \frac{\tau}{\Theta B} + \frac{x^{2\nu}(x^2-\rho^2)}{2(\rho^{2\nu+2}-1)} + \frac{\rho^2(\rho^{2\nu}-x^{2\nu})}{2\nu(\rho^{2\nu+2}-1)} + \frac{\rho^2(\rho^{2\nu}-1)x^{2\nu}(\nu+1)}{2\nu(\rho^{2\nu+2}-1)^2}\right.$$

$$\left.+ \frac{x^{2\nu}(\nu+1)(1-\rho^{2\nu+4})}{(2\nu+4)(\rho^{2\nu+2}-1)^2}\right] \tag{19b}$$

$$+ (Q-2\nu)x^{\nu}\pi \sum_{n=1}^{\infty} - 2\exp(\frac{-\alpha_n^2\tau}{\Theta B})\ F_\nu(x,\alpha_n) \tag{19c}$$

$$+ \frac{2\nu x^{\nu}}{\rho^{\nu+1}} \pi \sum_{n=1}^{\infty} - 2 \exp(\frac{-\alpha^2}{\Theta B}) \frac{J_{\nu+1}(\alpha) F_{\nu}(x,\alpha n)}{\alpha_n^2 \, J_{\nu+1}(\rho\alpha)} \qquad (19d)$$

Finally when transport is simply by diffusion and adsorption instantaneous:

$$U = 1 \quad + \qquad (20a)$$

$$+ Q\{\frac{2}{\rho^2-1} \frac{\tau}{\Theta B} + \frac{x^2-\rho^2}{2(\rho^2-1)} + \frac{\rho^2}{\rho^2-1} \ln(\frac{\rho}{x}) + \frac{\rho^2}{(\rho^2-1)^2} \ln\rho - \frac{(1+\rho^2)}{4(\rho^2-1)}\} + \qquad (20b)$$

$$+ Q\pi \sum_{n=1}^{\infty} - 2 \exp(\frac{-\alpha_n^2\tau}{\Theta B}) \frac{F_o(x,\alpha_n)}{\alpha_n^2} \qquad (20c)$$

When adsorption is instantaneous V = U at any time and distance.

3. RESULTS AND DISCUSSION

It is possible to draw some conclusions from equations (15-20) without actually performing any complicated calculations.

The solutions for U are composed of three ((17)and(20)) or four ((15) and (19))parts. The first part (part a) gives the steady-state situation when no uptake occurs (Q = 0). When transport is by diffusion only this steady-state situation is identical to the initial situation. When flow of water contributes to the transport of the solute and Q = 0, the concentration in the steady-state situation is a decreasing function of the distance, as the derivative of U with respect to x:

$$\frac{\delta U}{\delta x} = \frac{2\nu(\rho^2-1)}{\rho^{2\nu+2}-1}\,(\nu+1)x^{2\nu-1}$$

is negative for all x. In this situation the diffusion away from the root just cancels the transport by mass flow towards the root or:

$$\frac{\delta U}{\delta x} = \frac{-2\nu}{x}U$$

When $Q \neq 0$ the parts c and d sooner or later can be neglected, as time advances, since time in these components occurs solely in the exponent with a negative coefficient (s_{n_1} and s_{n_2}, and of course $-\alpha_n^2$ are negative), eventually thus only part a and b remain (the factor $(1-e^{-B\lambda\tau})$ in the last term of 15b and 17b will then equal unity). Where transport is by diffusion only the sum of a and b represents the steady-rate situation. This situation is characterized by the fact that the rate of decrease of U is independent of both time and distance:

$$\frac{\delta U}{\delta \tau} = \frac{2Q}{(\rho^2-1)B\Theta}$$

Once such a situation has developed the concentration profile will thus maintain its then established shape. When mass flow plays an important role in transport $\frac{\delta U}{\delta \tau}$ will eventually become independent of time but will nevertheless stay a function of distance:

$$\frac{\delta U}{\delta \tau} = \frac{2Q(\nu+1)x^{2\nu}}{(\rho^{2\nu+2}-1)\Theta B}$$

The contribution of mass flow to transport is governed by the parameter ν, the value of which both in absolute sense and in relation to the value of Q is important. Normally the value of ν is quite close to zero as the next simple calculation shows: for arable crops the root density (W) in the plow layer of about 20 cm (h), will usually not be much lower than 1 cm cm^{-3}, while for not too dry conditions the diffusion coefficient (D) can be expected to be about 0.1 $cm^2 day^{-1}$, thus with transpiration (E) of the order of 0.5 cm day^{-1}, ν will assume the value:

$$\nu = -0.5/(4 * \pi * 20 * 0.1 * 1) = -0.02$$

This implies that the first term of eq. (15) and (19) will deviate not too much (within 10%) from unity for all x. One can also expect the parts 15b and 19b not to differ too much from their equivalents in eq (17) and (20). The third component 15c and 19c will differ substantially from 17c and 20 if 2ν is of the same order as or greater than Q.

From the definitions of Q and ν it follows:

$$Q/2\nu = \frac{\rho^2}{2\eta\phi} \cdot \frac{2\eta\phi_w}{\rho^2} = \frac{D}{ER_0} \cdot \frac{AR_0}{DC_i} = \frac{A}{EC_i}$$

For a nutrient like phosphate the average uptake is 4-5 * 10^{-3} mg P cm^{-2} day^{-1} (based on a growth rate of 200 kg ha^{-1} day^{-1} and a P-content of 0.5% P_2O_5), and the concentration of P in the soil solution usually does not exceed 10^{-3} mg ml^{-1}.

Transpiration being 0.3-0.5 cm day^{-1}, the ratio $Q/2\nu$ according will be of the order:

$$Q/2\nu = 10 - 15$$

In the coefficient $(Q-2\nu)$ of the infinite series in eq 15c and 19c consequently 2ν can in a first approximation be neglected with respect to Q. For a nutrient like nitrate on the other hand rate of uptake amounts to 3 * 10^{-2} mg cm^{-2} day^{-1} based on 200 kg DM ha^{-1} day^{-1} and N content of 1.5%

and concentration in the soil solution, when sufficient nitrate is present to ensure good crop growth is about 0.8 mg ml^{-1}, so $Q/2\nu$ assumes the value: 0.075. In this case Q is of the same order or even smaller than 2ν, and considerable difference can be expected to occur between 15c and 19c, or 17c and 20c.

Calculation of values of U (and V) when the infinite series cannot be ignored, requires the use of a computer. In Appendix III the main features of the computer programs employed are explained. Calculations were done for two types of solute, one of which is subject to adsorption ("phosphate") and one which is not ("nitrate"). The range of the parameter values is given in table I.

TABLE I. Range of values of parameters used in the calculations.

Variable	Symbol	Dimension	Range
Transpiration	E	cm day^{-1}	0 - 1
Adsorption constant	K	ml cm^{-3}	0(nitrate) 100 (phosphate)
Water content	Θ	ml cm^{-3}	0.25
Diffusion coefficient	D	cm^2 day^{-1}	0.1
Root density	W	cm^{-2}	0.5-5
Half time adsorption rate	$t_{\frac{1}{2}}$	day	0-30
Initial concentration	C_i	mg ml^{-1}	10^{-3} (P) - 0.8 (N)
Uptake rate	A	mg cm^{-2} day^{-1}	4.4×10^{-3}(P)-$3\text{x}10^{-2}$(N)
Root radius	R_o	cm	0.025
Plow layer (root length)	h	cm	20
Root absorbing power	m	cm day^{-1}	0.043-0.43 (nitrate) 6.5 - 56 (phosphate)

If not explicitly mentioned otherwise, the results exhibited pertain to a root density of 1 cm cm^{-3}.

First the influence of mass flow when adsorption is instantaneous will be discussed. Fig. 3 shows the development of the concentration profile

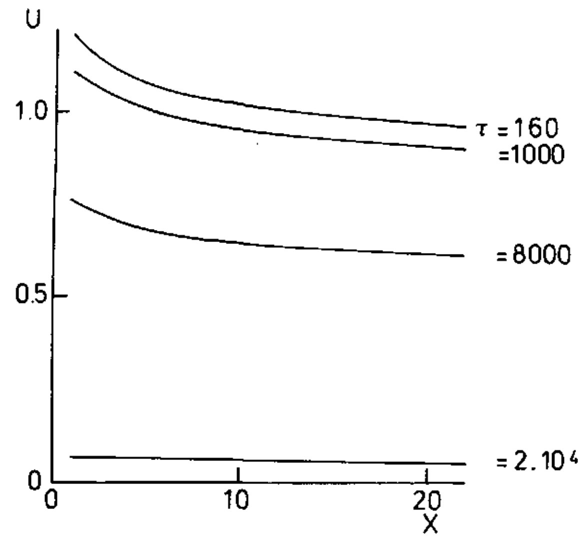

Fig. 3a. Nitrate concentration as function of distance and time. Transpiration 1 cm day^{-1}.

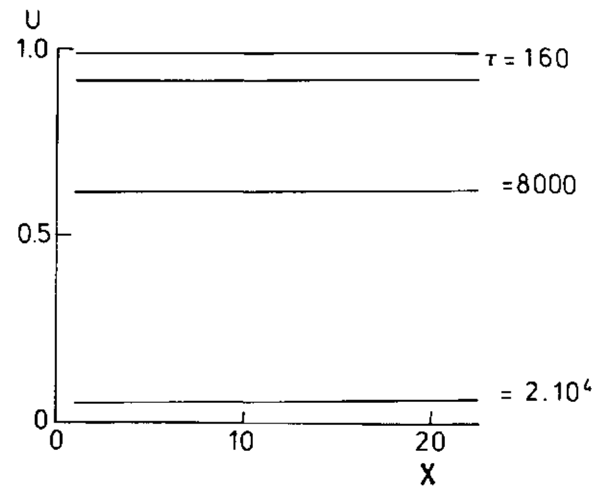

Fig. 3b. As fig. 3a. Transpiration 0 cm day^{-1}.

around the root with time for nitrate, when transpiration is high (E = 1 cm day^{-1}, fig. 3a) and when it is absent (fig. 3b).When mass flow is occuring one can see that almost up to the time of total depletion of the soil cylinder, concentration is a decreasing function of distance (fig. 3a). When diffusion alone is responsible for transport almost no gradients develop, as - because of the relatively high diffusion coefficient - very small gradients suffice to meet the uptake rate of the root. Moreover very soon (in about 1 day) the series part of the solutions become negligible and concentration becomes a linear function of time, as is shown in fig. 4.

In the case of phosphate at any time the lowest concentrations are found at the root surface, the highest concentrations, however, are not always situated at the outer boundary of the soil cylinder. At high transpiration rate a situation may develop in which the concentration passes through a maximum somewhere in the soil cylinder. Such a maximum, albeit not very pronounced, can be found in fig. 5a, in the curve for τ = 16000 where concentration is at a maximum for x = 18. The steady-rate situation is attained much later in the case of phosphate than in the case of nitrate, because the coefficient of τ in the exponent in

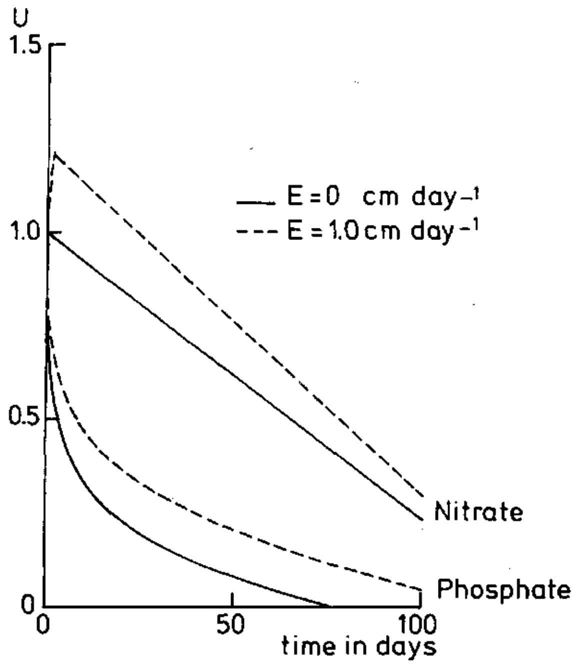

Fig. 4. Time course of concentration of nitrate and phosphate at root surface.

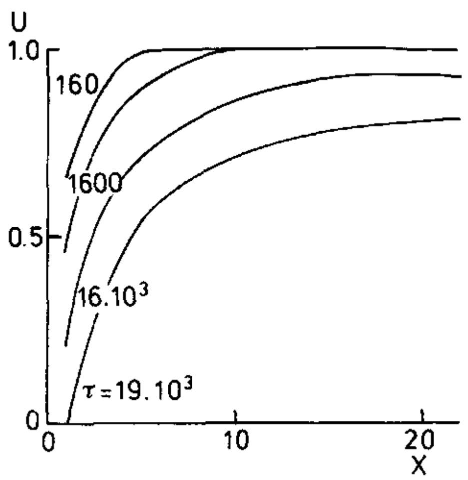

Fig. 5a. Phosphate concentration as function of distance and time. Transpiration 1 cm day^{-1}.

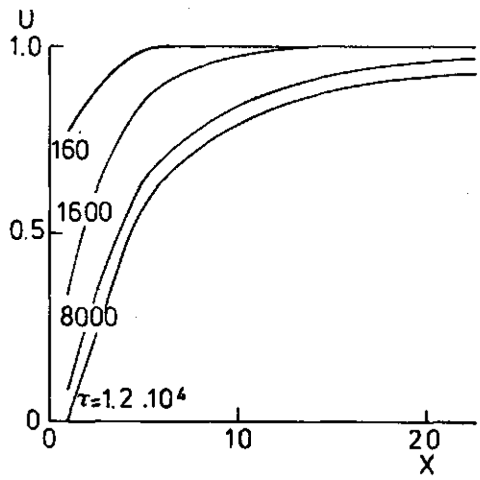

Fig. 5b. As fig. 5a. Transpiration 0 cm day^{-1}.

the infinite series (20c) is proportional to the reciprocal buffer capacity B.

It is interesting to analyze in which way the various components of equation 19 contribute to the value of U. Fig. 6 shows these components as function of distance for two different times in the case of phosphate and a transpiration of 1 cm day^{-1}. As can be seen the components containing the series (c an d) play a less prominent role as time proceeds. (For τ = 3200 part d can not be shown in fig. 6, as its maximal value is approximately 0.01). Ultimately only part a (which is invariable with time) and part b remain. An important characterization of the possibilities of the soil-root system with respect to uptake is given by the period during which the concentration at the root surface exceeds the limiting concentration. During this period - denoted by the symbol τ_c - uptake of the root is completely in accordance with the demand of the plant. If it may be assumed that when τ equals τ_c, the series part of (19) and (20) can be neglected, it is easy to make τ_c explicit:

$$\tau_c = \frac{\Theta B(\rho^{2\nu+2}-1)}{2(\nu+1)\,Q}\,U_1 - \frac{\Theta B(\rho^2-1)}{2Q} +$$

$$- \frac{\Theta B}{2(\nu+1)}\left\{\frac{1-\rho^2}{2} + \frac{\rho^2(\rho^{2\nu}-1)}{2\nu} + \frac{\rho^2(\rho^{2\nu}-1)}{2\nu(\rho^{2\nu+2}-1)} + \frac{(1-\rho^{2\nu+4})}{(2\nu+4)(\rho^{2\nu+2}-1)}\right\} \qquad (21)$$

or when transport is by diffusion only:

$$\tau_c = \frac{\Theta B(\rho^2-1)}{2Q}\,(U_1-1) - \frac{\Theta B}{2}\left\{\frac{1-\rho^2}{2} + \rho^2\ln\rho + \frac{\rho^2\ln\rho}{\rho^2-1} - \frac{(\rho^2+1)}{4}\right\} \qquad (22)$$

In (21) and (22) U is the dimensionless limiting concentration ($U_1 = C_1/C_i$). For nitrate steady rate is reached very soon (within a day, see fig. 3), so that for all root densities τ_c can be calculated with (21) or (22). The same is true for phosphate if the root-density is greater than or equal to 1 cm^{-2}. If C_1 is zero the maximum period of unconstrained uptake is given by:

$$t_{max} = \frac{\int_{R_1}^{R_0} 2\pi r h(K+\Theta)C\,dr}{\pi R_1^2 A} = \frac{h(R_1^2-R_0^2)}{R_1^2 A}\,(\Theta+K)C_i$$

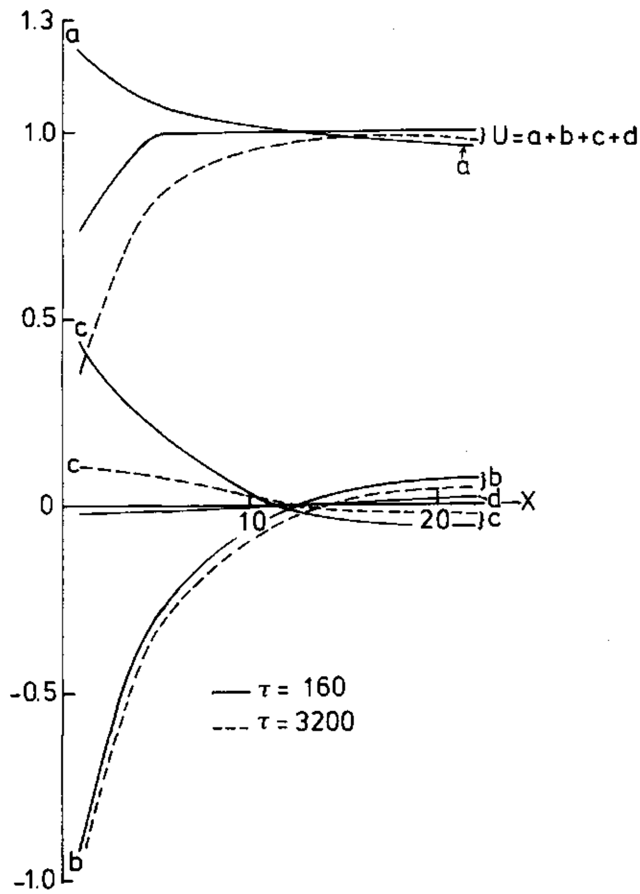

Fig. 6. Contribution of the four terms of equation (19) to the concentration U.

or in dimensionless form:

$$\tau_{max} = \frac{Dt_{max}}{R_0^{\,2}} = \Theta B\phi\eta\left(\frac{\rho^2-1}{\rho^2}\right) \tag{23}$$

The realized fractional depletion (F_d) is given by:

$$F_d = \frac{\tau_c}{\tau_{max}} \tag{24}$$

In fig. 7 F_d is given as a function of root-density for the two rates of transpiration, 0 and 1 cm day^{-1}. In the case of nitrate the curves for zero transpiration and transpiration of 1 cm day^{-1} practically coincide with the line of total depletion, which means that even without any contribution to transport by mass flow a rather sparse root system with root-density 0.5 cm^{-2} can take up almost all the available nitrogen at the required rate. For phosphate transport by mass flow can considerably lengthen the period of unconstrained uptake, or increase the fractional depletion. Fig. 7 shows that at a root-density of 1 cm cm^{-3} F_d (and so τ_c) is increased with a factor 1.5 when transpiration is 1 cm day^{-1}.

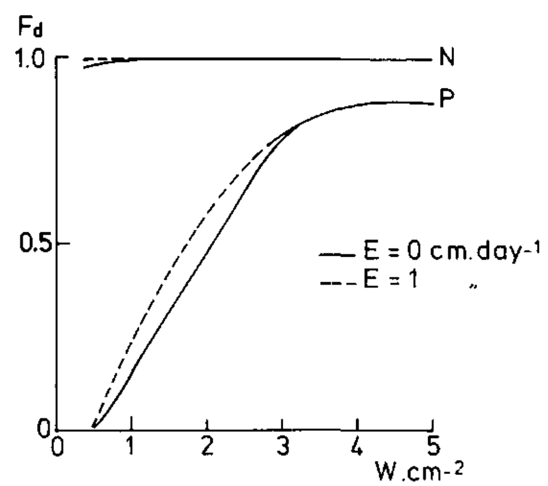

Fig. 7. Fractional depletion (F_d) of nitrate and phosphate when U (1, τ) = 0 as function of root density (W).

If U_1 is greater than zero it would seem obvious to define τ_{max} as:

$$\tau_{max} = \Theta B\eta(\frac{\rho^2-1}{\rho^2})(\phi-\phi_1) \qquad (25)$$

with $\phi_1 = \frac{DC_1}{AR_0}$. But this definition bears the disadvantage that for some values of U_1, F_d would be greater than 1. If for example $U_1 = 0.75$ it follows from fig. 3a that τ_c is approximately 8000 while τ_{max} calculated according to (25) amounts to 5300. To overcome this difficulty τ_{max} was defined as in (24) even when $U_1 > 0$.

As was explained earlier (section 2) C_l and so U_l is in fact a function of root-density:

$$U_l = C_l/C_i = \frac{\rho^2}{2\eta\mu}, \text{ where } \mu = \frac{mC_i}{A}$$

Nye and Tinker (1977) give values of m (α in their notation) ranging from $2.5 * 10^{-2}$ - 2 cm day^{-1} (for nitrate) and from 6.5-56 cm day^{-1} (for phosphate). In fig. 8a and b the fractional depletion is given as function of root density and root absorbing power. Again it is shown that mass flow can considerably increase depletion in case of phosphate, while for nitrate except for very low root-densities and root absorbing power, the increase in depletion due to mass flow amounts to a few per cent.

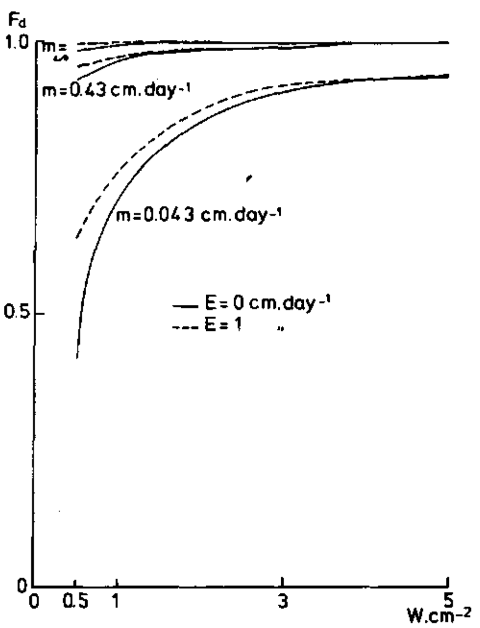

Fig. 8a. Fractional depletion (F_d) of nitrate as function of root-density and root absorbing power.

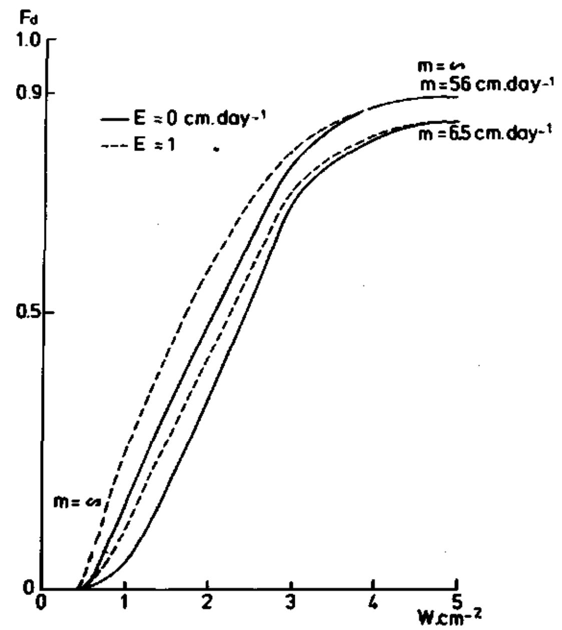

Fig. 8b. As fig. 8a for phosphate.

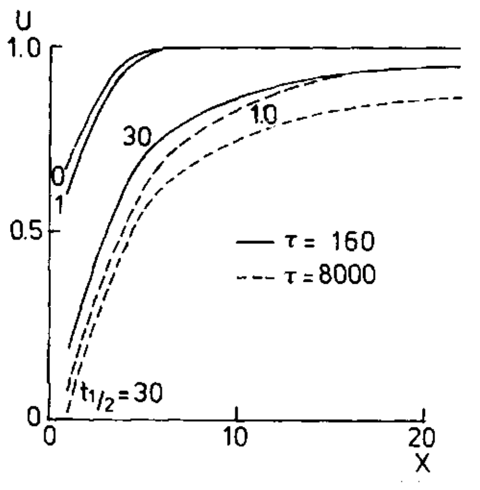

Fig. 9a. Concentration as function of distance and time for different half-life values of the adsorption reaction (the numbers at the curves). Transpiration 1cm day^{-1}.

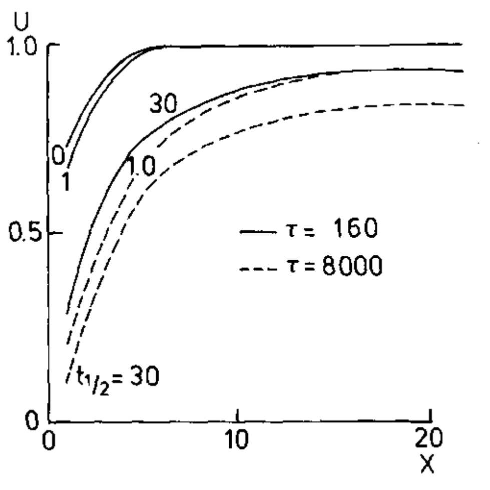

Fig. 9b. As fig. 9a. Transpiration 0 cm day^{-1}.

Comparison of the effects of finite rate of adsorption with instantaneous adsorption is of course only relevant in the case of phosphate. Fig. 9a and 9b show the concentration as a function of the distance at some points of time for various half-life values of the adsorption reaction. The profiles for $t_{\frac{1}{2}}$ = 0 and $t_{\frac{1}{2}}$ = 1 day coincide except for short times. For half-life values of the order of a month the concentration of course decreases much faster. In fig. 10 both U and V are plotted for the high half-life periods ($t_{\frac{1}{2}}$ = 30 days). In the beginning (t = 1 , or τ = 160) the rate of desorption is small which leads to a sharp decrease in concentration in the vicinity of the root. This low concentration enhances the desorption rate (cf.eq.(6)) and the concentration in the soil solution is replenished by the adsorbed phase. In fig. 11 the time course of the concentration at the root surface is given for transport by diffusion only, and for transport by diffusion and mass flow. Once more the rapid initial reduction in concentration is manifest, followed by a much slower decrease. For reference, the curve for instantaneous adsorption is included in fig. 11. To analyze the curves for transport by diffusion the development in time of the components a, b, and c is shown in fig. 12. The immediate decrease of part c

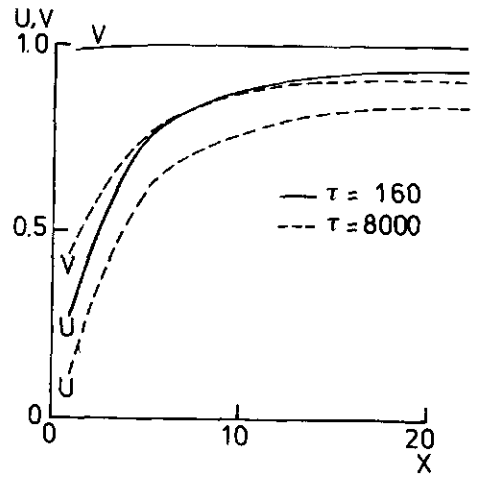

Fig. 10. Concentration in soil solution (U) and in the adsorbed phase (V) as function of distance and time. Half-life adsorption reaction 30 days. Transpiration 1 cm day^{-1}.

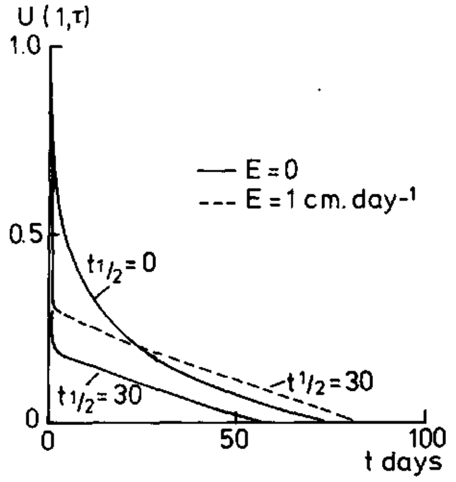

Fig. 11. Time course of the concentration at the root surface for finite and infinite rate of adsorption, and two transpiration rates.

is greater when the adsorption half time is 30 days (the value at $\tau = 0$ is 0.83 both for finite and infinite rate of adsorption), but later on (after 25 days) the situation is reversed. In case of instantaneous adsorption part b is a linear function of τ, for finite adsorption rate

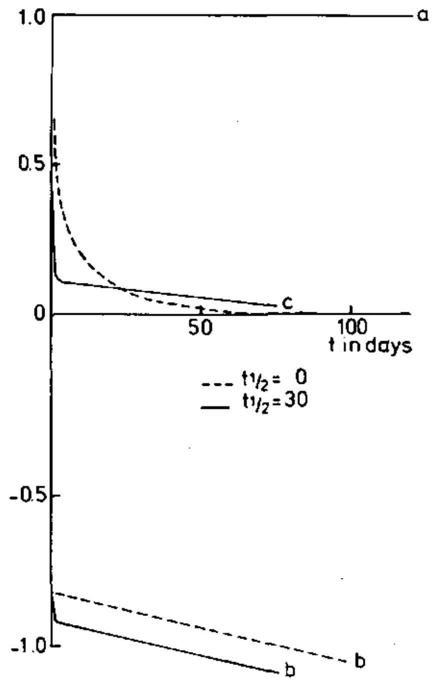

Fig. 12. Contribution of the three terms of equation(17) to the concentration U.

initially the term with factor $(1-e^{-B\lambda\tau})$ (see eq. 17b) is of some importance, very soon this factor approximates unity. Thus from t = 1 (τ = 160) a constant difference is maintained with part b in case of instantaneous adsorption. In fig. 13 the concentration in the adsorbed phase V is plotted. In a way, this figure is a reflection of fig. 9b. It shows the smaller decrease of V when the adsorption rate constant is lower. Fig. 14 shows a plot of Tx (see section 2 for definition of T) versus x for finite and infinite adsorption rate. The depletion is proportional to the difference between the area under the line y = x, and the curve y = Tx, as T initially is unity for all x . It is evident from this figure that depletion at a given time is the same for both values of the adsorption rate constant, as it should be.

Analogous to eq. (21) and (22) the period of unconstrained uptake τ_c can be given as explicit function of ρ and the other parameters, if at least the parts c and d of equation (15) and (17) can be neglected:

$$\tau_c = \frac{-(B-1)}{B\lambda} + \frac{\Theta\ B(\rho^{2\nu+2}-1)}{2(\nu+1)Q}\ U_1 - \frac{\Theta B(\rho^2-1)}{2Q} +$$

$$- \frac{\Theta B}{2(\nu+1)}\ \{ \frac{1-\rho^2}{2} + \frac{\rho^2(\rho^{2\nu}-1)}{2\nu} + \frac{\rho^2(\rho^{2\nu}-1)}{2\nu(\rho^{2\nu+2}-1)} + \frac{1-\rho^{2\nu+4}}{(2\nu+4)(\rho^{2\nu+2}-1)} \qquad (26)$$

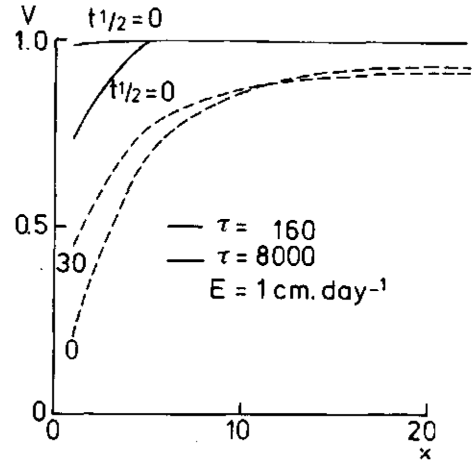

Fig. 13. Concentration of adsorbed solute (V) as function of time and distance, for finite and infinite adsorption rate.

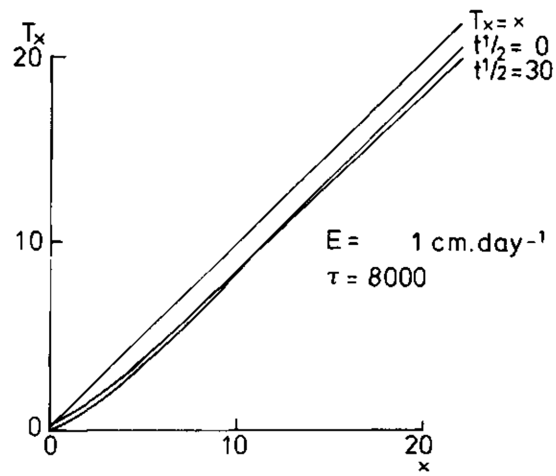

Fig. 14. Plot of the product of distance (x) and bulk density of solute (T) versus distance for finite and infinite adsorption rate.

or when $\nu = 0$

$$\tau_c = \frac{-(B-1)}{B\lambda} + \frac{\Theta B}{2Q}(\rho^2-1)(U_1-1) - \frac{\Theta B}{2}\left\{\frac{1-\rho^2}{2} + \rho^2 \ln\rho + \frac{\rho^2 \ln\rho}{\rho^2-1} - \frac{(\rho^2+1)}{4}\right\} \quad (27)$$

Compared with (21) and (22), (26) and (27) show that, since $B \gg 1$, τ_c is shortened by a period $1/\lambda$ when adsorption is non-instantaneous.

But this is only the case if (quasi) steady-rate is reached before the concentration at the root surface attains U_1. As shown in fig. 11 and 12 this is for instance not the case when the adsorption half-life is 30 days, and root-density is 1 cm^{-2}, as part c contributes significantly to U, up to the time U (1, τ) becomes zero, rendering a calculation of τ_c with equation (27) incorrect. In fig. 15 the fractional depletion F_d is plotted as function of root density and root absorbing power for $t_{\frac{1}{2}}$ = 30 days. This figure of course bears a close resemblance to fig. 5, be it that the effect of mass flow is smaller for high and greater for low root absorbing power. If calculation of τ_c (and so of F_d) with eq. (26) or (27) is justified the difference in F_d between instantaneous and non instantaneous adsorption is given by $1/(\lambda\tau_{max})$ or with the parameter values employed here, F_d should be 0.096 greater when adsorption is instantaneous. Comparison of fig. 15 with fig. 7 shows that this is only the case for higher root densities.

Summarizing, the most important conclusions seem to be that normally transport by mass flow of nitrate to the plant root does not significantly enhance the possibilities of a root system to deplete the soil of the available nitrogen (fig. 7 and 8a). The diffusion mechanism alone is sufficient to bring nitrate to the root at the required rate. A similar conclusion, but for the root to behave as a zero sink, was formulated by Van Keulen *et al.* (1975). On the other hand, for a nutrient like phosphate which is strongly buffered and the concentration of which in the soil solution is (very) low, transport by mass flow can, depending on root density, considerably increase the depletion. Another conclusion is that when the adsorption/desorption reaction is completed within a few days, as is usually the case with phosphate (Beek, 1979; Barrow, 1975), it is fully justified to consider adsorption instantaneous, as far as transport to and uptake by a root is concerned, as was done a.o. by Van Noordwijk *et al.* (in preparation). When realistic values are attached to the parameters, as was done as much as possible here, the absolute value of the mass flow parameter 2ν will not exceed 0.1, so choosing - for computational convenience - a value of -0.5 for 2ν as was done by Cushman (1979b) would imply either an unrealistic high value of the transpiration, or an equally unrealistic low value of the root density.

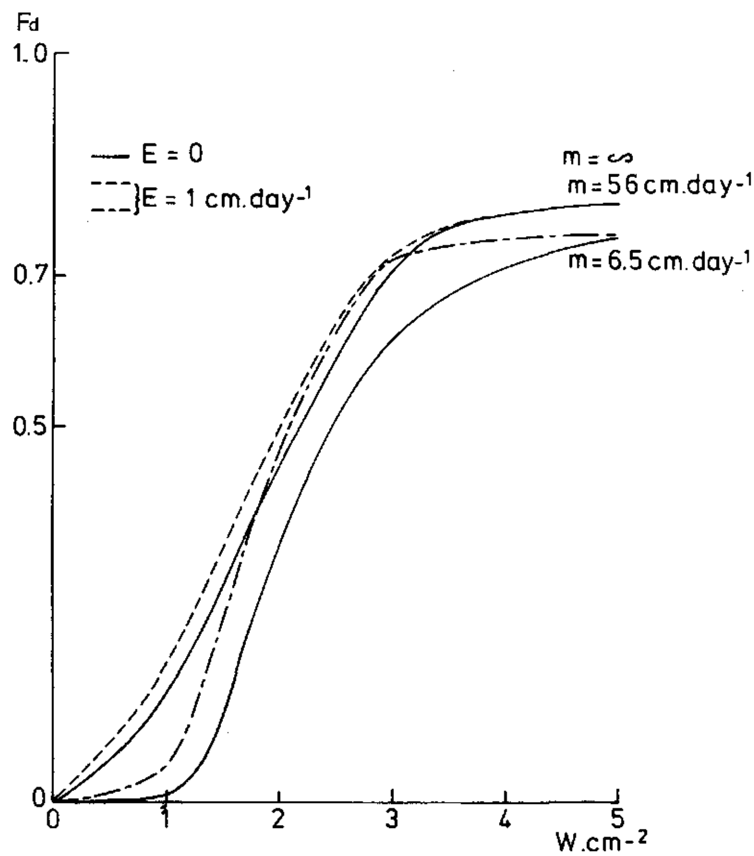

Fig. 15. Fractional depletion as function of root-density and root absorbing power. Half-life adsorption reaction is 30 days.

Another difference of Cushman's treatment with the approach employed here lies in the choice of the boundary condition at the root surface. Following Nye and Marriot (1969), Cushman (1979a) assumes uptake to be proportional to solute concentration at the root wall. This can lead to very high uptake rates, when high root densities are taken into consideration, because doubling the root density would mean, at least initially, doubling the uptake rate of the crop per cm^2 soil.

Whether one chooses one boundary condition or the other, generally, a formidable number of assumptions, idealizations, and simplifications have to be used in order to arrive at an analytical solution at all. A good deal can be learnt from (the derivation of) analytical solutions, even though these can only be found for biologically or agronomically rather unrealistic or trivial situations (linear adsorption, zero or first order rate kinetics, simple uptake mechanisms etc.). Even for such oversimplified conditions, the solutions derived are often complex, and the complete calculation requires the use of a computer. In those cases where one is interested in a specific situation, it would seem advisable to use numerical methods even when theoretically an analytical solution is possible.On the other hand the approach followed in this paper, in particular the use of dimensionless variables, allows a larger degree of generalization of the results.

4. SUMMARY

An analytical solution concerning diffusion and mass flow of a solute to a root, when uptake is constant and when adsorption or desorption of the solute by the soil proceeds at finite rate, is presented. From this solution, solutions could be derived for instantaneous adsorption and/or transport by diffusion only. The concept of a limiting concentration above which root uptake is independent of concentration and proceeds conform to the demand of the plant is discussed. Results of calculations are presented, pertaining to two types of solute, one which is subject to adsorption (phosphate) and one which is not (nitrate). It is shown that the period of uptake, in accordance with plant demand, is not significantly increased when in addition to diffusion mass flow contributes to transport of the solute, as far as nitrate is concerned. In case of phosphate mass flow can, at not too high root-densities, considerably lengthen the period of uptake according to plant demand. When the half-life value of the adsorption reaction is of the order of a few days, it is shown that the development of the concentration profile is virtually identical to that developed when adsorption is instantaneous.

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APPENDIX I

The solution of equations (10) and (11) subject to conditions (12),(13) and (14) is obtained by the Laplace transformation denoted by L { }

If

$L\{U\} = u$

$L\{V\} = v$

and transformation is taken with respect to τ, the Laplace parameter being denoted by s, then (10)-(13) with initial condition (14) transform into:

$$K(sv-1) + \Theta(su-1) = \frac{d^2u}{dx^2} + \frac{1}{x}(1-2\nu)\frac{du}{dx} \tag{A-1}$$

$$sv-1 = \lambda(u-v) \tag{A-2}$$

$$\text{for } x = \rho:\ -\frac{\delta u}{\delta x} + \frac{2\nu}{\rho}u = 0 \tag{A-3}$$

$$\text{for } x = 1:\ -\frac{\delta u}{\delta x} + 2\nu u = \frac{Q}{s} \tag{A-4}$$

From (A-2): $v = \frac{\lambda}{s+\lambda}u + \frac{1}{s+\lambda}$

Substituting the result in the lefthand side of (A-1) one gets:

$$\beta u - \frac{\beta}{s} = \frac{du^2}{dx^2} + \frac{1}{x}(1-2\nu)\frac{du}{dx} \tag{A-5}$$

with $\beta = \frac{K\lambda s}{s+\lambda} + \Theta s = \frac{\Theta s(s+B\lambda)}{s+\lambda}$ where $B = \frac{K+\Theta}{\Theta}$

The solution of the homogeneous part of (A-5) is given by Abramowitz and Stegun (1970), (page 362, 9.1.52):

$$u_h = c_1 x^{\nu} I_{\nu}(x\sqrt{\beta}) + c_2 x^{\nu} K_{\nu}(x\sqrt{\beta})$$

where I_ν and K_ν are modified Besselfunctions of first resp. second kind and order ν.

A particular solution of (A-5) is:

$$u_p = \text{constant}$$

The general solution is given by:

$$u = u_p + u_h$$

By substitution of u in (A-5) it is found that: $u_p = \frac{1}{s}$

The solution of (A-5) is thus given by:

$$u = \frac{1}{s} + c_1 x^{\nu} I_{\nu}(x\sqrt{\beta}) + c_2 x^{\nu} K_{\nu}(x\sqrt{\beta}) \qquad \text{(A-6)}$$

The constants c_1 and c_2 are found from the boundary conditions.
The derivative of u with respect to x is: (App. II p11 and p12 *))

$$\frac{du}{dx} = c_1 x^{\nu}\sqrt{\beta} I_{\nu-1}(x\sqrt{\beta}) - c_2 x^{\nu}\sqrt{\beta} K_{\nu-1}(x\sqrt{\beta}) \qquad \text{(A-7)}$$

Substituting (A-7) and (A-6) in (A-3) and (A-4) and using properties p6 and p7 leads to

$$c_2\sqrt{\beta} K_{\nu+1}(\sqrt{\beta}) - c_1\sqrt{\beta} I_{\nu+1}(\sqrt{\beta}) = -\frac{Q-2\nu}{s} \qquad \text{(A-8)}$$

$$c_2 \rho^{\nu}\sqrt{\beta} K_{\nu+}(\rho\sqrt{\beta}) - c_1 \rho^{\nu}\, \beta I_{\nu+1}(\rho\sqrt{\beta}) = \frac{-2\nu}{\rho s} \qquad \text{(A-9)}$$

Solving for c_1 and c_2 results in:

---

*) In Appendix II some properties of Besselfunctions are given relevant for the derivation treated here. These properties will from here on be referred to as p1, p2, etc.

$$c_1 = \frac{(2\nu-Q)\rho^{\nu}K_{\nu+1}(\rho\sqrt{\beta}) - 2\nu K_{\nu+1}(\sqrt{\beta})/\rho}{s\sqrt{\beta}\rho^{\nu}\{K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta})\}}$$

$$c_2 = \frac{(2\nu-Q)\rho^{\nu}I_{\nu+1}(\rho\sqrt{\beta}) - 2\nu I_{\nu+1}(\sqrt{\beta})/\rho}{s\sqrt{\beta}\rho^{\nu}\{K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta})\}}$$

So that eventually the solution for u is given by:

$$\begin{aligned} u = {} & \frac{1}{s} + \\ & + \frac{(2\nu-Q)x^{\nu}\{K_{\nu+1}(\rho\sqrt{\beta})I_{\nu}(x\sqrt{\beta}) + I_{\nu+1}(\rho\sqrt{\beta})K_{\nu}(x\sqrt{\beta})\}}{s\sqrt{\beta}\{K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta})\}} + \\ & - \frac{2\nu x^{\nu}\{K_{\nu+1}(\sqrt{\beta})I_{\nu}(x\sqrt{\beta}) + I_{\nu+1}\ \beta)K_{\nu}(x\sqrt{\beta})\}}{s\sqrt{\beta}\rho^{\nu+1}\{K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta})\}} \end{aligned} \qquad \text{(A-9)}$$

The concentration U can thus be found as the inverse Laplace transform of u given by (A-9).

Let the three terms of the RHS of (A-9) be denoted by u_I, u_{II}, and u_{III} respectively.

The inverse of u_I is found straight forwardly:

$$U_I = L^{-1}\{u_I\} = 1 \qquad \text{(A-10)}$$

The inverse transform of u_{II} and u_{III} can be found by interpreting the Laplace parameters as a complex variable, and using the complex inversion integral (Churchill (1972)):

$$U_{II} = L^{-1}\{u_{II}\} = \frac{1}{2\pi i}(2\nu-Q)x^{\nu} \ast$$

$$\int_{\gamma-i\infty}^{\gamma+i\infty} \frac{K_{\nu+1}(\rho\sqrt{\beta})I_{\nu}(x\sqrt{\beta}) + I_{\nu+1}(\rho\sqrt{\beta})K_{\nu}(x\sqrt{\beta})}{\{K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta})\}s\sqrt{\beta}} e^{s\tau} ds$$

The value of the integral can be found as the sum of the residues at the poles of the integrand. It can be seen easily that $s = 0$ is a singular point of the integrand.
To investigate the order of the pole $s = 0$ the numerator of the integrand is written as (omitting the factor $e^{s\tau}$)

$$I_\nu(x\sqrt{\beta})K_{\nu+1}(\rho\sqrt{\beta}) + K_\nu(x\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta}) =$$

$$\frac{\pi}{2\sin\nu\pi}\{I_{-\nu}(x\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta}) - I_\nu(x\sqrt{\beta})I_{-(\nu+1)}(\rho\sqrt{\beta})\} \qquad \text{(A-11)}$$

In deriving (A-11) use is made of the definition of K_ν (p5).
If next the Besselfunctions I are written as infinite series (p4) and the terms are rearranged (A-11) becomes

$$\frac{\pi}{2\sin\nu\pi}\cdot\frac{1}{\sqrt{\beta}}\{\frac{x^{-\nu}\rho^{\nu+1}\beta}{2\Gamma(\nu-1)\Gamma(\nu+2)} - \frac{2x^\nu\rho^{-(\nu+1)}}{\Gamma(\nu+1)\Gamma(-\nu)} - \frac{x^{\nu+2}\rho^{-(\nu+1)}\beta}{\Gamma(\nu+1)\Gamma(-\nu)(2+2\nu)} +$$

$$+ \frac{x\rho^{1-\nu}\beta}{2\nu\Gamma(\nu+1)\Gamma(-\nu)} + 0(\beta^2)\}$$

Where $0(\beta^2)$ stands for all terms in β of order two and higher.

Likewise the denominator can be written:

$$K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta}) =$$

$$s\sqrt{\beta}\frac{\pi}{2\sin\nu\pi}\left[\frac{\rho^{\nu+1}-\rho^{-(\nu+1)}}{\Gamma(\nu+2)\Gamma(-\nu)} + \{\frac{\rho^{\nu+3}-\rho^{-(\nu+1)}}{\Gamma(\nu+2)\Gamma(-\nu)(2\nu+4)2} - \frac{\rho^{\nu+1}+\rho^{1-\nu}}{4\nu\Gamma(\nu+2)\Gamma(-\nu)}\}\beta + 0(\beta^2)\right]$$

The integrand accordingly can be written in the form:

$$\frac{e^{s\tau}}{s\beta}\{\frac{a_1+a_2\beta+0(\beta^2)}{b_1+b_2\beta+0(\beta^2)}\}$$

where $a_1 = \frac{-2x^\nu\rho^{-(\nu+1)}}{\Gamma(\nu+1)\Gamma(-\nu)}$

$$a_2 = \frac{\rho^{\nu+1}x^{-\nu}}{2\Gamma(1-\nu)\Gamma(\nu+2)} + \frac{\rho^{1-\nu}x^\nu}{2\nu\Gamma(\nu+1)\Gamma(-\nu)} - \frac{x^{\nu+2}\rho^{-(\nu+1)}}{\Gamma(\nu+1)\Gamma(-\nu)(2+2\nu)}$$

$$b_1 = \frac{\rho^{\nu+1}-\rho^{-(\nu+1)}}{\Gamma(\nu+2)\Gamma(-\nu)}$$

$$b_2 = \frac{\rho^{\nu+3}-\rho^{-(\nu+1)}}{\Gamma(\nu+2)\Gamma(-\nu)2(2\nu+4)} - \frac{\rho^{\nu+1}+\rho^{(1-\nu)}}{4\nu\Gamma(\nu+2)\Gamma(-\nu)}$$

or using the definition of β given earlier:

$$\frac{e^{s\tau}(s+\lambda)}{\Theta s^2(s+B\lambda)} \left\{ \frac{a_1+a_2\beta+0(\beta^2)}{b_1+b_2\beta+0(\beta^2)} \right\} \qquad \text{(A-12)}$$

From (A-12) it can be seen that $s = 0$ is a double pole.
Let (A-12) be symbolized by $F(s)$ then, using
$\left.\frac{d\beta}{ds}\right|_{s=0} = \Theta B$ en $\beta|_{s=0} = 0$, the residue at the pole $s = 0$
is given by (Churchill(1970)):

$$\lim_{s\to 0} \frac{d}{ds}\, s^2F(s) = \frac{a_1}{\Theta b_1}\frac{\tau}{B} + \frac{a_1}{\Theta b_1}\frac{1}{B\lambda} + \frac{a_2}{b_1} - \frac{a_1}{\Theta b_1 B^2\lambda} - \frac{a_1 b_2}{b_1{}^2}$$

Also (A-12) shows $s = -B\lambda$ to be a single pole which residue is given by:

$$\lim_{s\to -B\lambda} (s+B\lambda)F(s) = \frac{e^{-B\lambda\tau}(1-B)}{\Theta B^2\lambda} \cdot \frac{a_1}{b_1}$$

Finally the integrand has poles for the zeros of

$$K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta}) = 0$$

This expression can be written using the properties p4 and p6 as:

$$Y_{\nu+1}(i\rho\sqrt{\beta})\ J_{\nu+1}(i\sqrt{\beta}) - Y_{\nu+1}(i\sqrt{\beta})\ J_{\nu+1}(i\rho\sqrt{\beta}) = 0$$

The zeros of $Y_{\nu+1}(\rho x)J_{\nu+1}(x) - Y_{\nu+1}(x)J_{\nu+1}(\rho x)$
are all real and simple (Abramowitz & Stegun, 1970).
Let them be denoted by $\alpha_n (n = 1, 2, 3, \ldots)$, then the integrand
has simple poles for $\beta = -\alpha_1^2, -\alpha_2^2, \ldots\ldots,$

or when s assumes the values:

$$s_{n_1} = \frac{-(B\lambda\Theta+\alpha_n^{\;2}) + \sqrt{(B\lambda\Theta+\alpha_n^{\;2})^2 - 4\lambda\alpha^2_{\;n}}}{2\Theta} \qquad \text{(A-13)}$$

$$s_{n_2} = \frac{-(B\lambda\Theta+\alpha_n^{\;2}) - \sqrt{(B\lambda\Theta+\alpha^2_{\;n})^2 - 4\lambda\alpha^2_{\;n}}}{2\Theta} \qquad \text{(A-14)}$$

The residues for these poles can be found as (Churchill)

$$\left[\frac{e^{-s\tau}}{s\sqrt{\beta}} \; \frac{\{K_{\nu+1}(\rho\sqrt{\beta})I_\nu(x\sqrt{\beta}) + I_{\nu+1}(\rho\sqrt{\beta})K_\nu(x\sqrt{\beta})\}}{\frac{d}{ds}\{K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta})\}}\right]_{\beta = -\alpha^2_{\;n}} \qquad \text{(A-15)}$$

Using the properties p9 and p10 and the fact that for

$$\beta = -\alpha^2_{\;n} \; : K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta}) = 0$$

the residue for $\beta = -\alpha^2_{\;n}$ becomes

$$2F_{II}(x,\rho,\alpha)\left[\frac{e^{s_{n_1}\tau}(s_{n_1}+\lambda)^2}{\Theta s_{n_1}\{(s_{n_1}+\lambda)^2 + (B-1)\lambda^2\}} + \frac{e^{s_{n_2}\tau}(s_{n_2}+\lambda)^2}{s_{n_2}\{(s_{n_2}+\lambda)^2 + (B-1)\lambda^2\}}\right]$$

with $F_{II}(x,\rho,\alpha) = \dfrac{K_{\nu+1}(\rho i\alpha)I_\nu(xi\alpha) + I_{\nu+1}(\rho i\alpha)K_\nu(xi\alpha)}{I_\nu(i\alpha)K_{\nu+1}(i\rho\alpha)+K_\nu(i\alpha)I_{\nu+1}(i\rho\alpha)-\rho\{I_{\nu+1}(i\alpha)K_\nu(\rho i\alpha)-I_\nu(\rho i\alpha)K_{\nu+1}(i\alpha)\}}$

Using the properties p4, p6, and p13 and repeatedly

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

the denominator of $F_{II}(x,\rho,\alpha)$ eventually becomes:

$$\frac{i}{\alpha} \cdot \frac{J^2_{\;\nu+1}(\alpha) - J^2_{\;\nu+1}(\rho\alpha)}{J_{\nu+1}(\alpha) \cdot J_{\nu+1}(\rho\alpha)}$$

and the numerator can be likewise transformed into

$$\frac{\pi i}{2}\{\, Y_{\nu+1}(\rho\alpha)J_{\nu}(\alpha x) - Y_{\nu}(\alpha x)J_{\nu+1}(\rho\alpha)\}$$

$F_{II}(x,\rho,\alpha)$ can thus be given as

$$F_{II}(x,\rho,\alpha) = \frac{\alpha\pi}{2}J_{\nu+1}(\alpha)J_{\nu+1}(\rho\alpha)\,\frac{\{J_{\nu}(\alpha x)Y_{\nu+1}(\rho\alpha) - Y_{\nu}(\alpha x)J_{\nu+1}(\rho\alpha)\}}{\{J^2_{\nu+1}(\alpha) - J^2_{\nu+1}(\rho\alpha)\}}$$

Thus the inverse of u_{II} is:

$$U_{II} = L^{-1}\{u_{II}\} = (Q-2\nu)\Bigg[\frac{2(\nu+1)x^{2\nu}}{\rho^{2\nu+1}-1}\cdot\frac{\tau}{\Theta B} - \frac{\rho^2\{(\nu+1)x^{2\nu}-\rho^{2\nu}\}}{2\nu(\rho^{2\nu+2}-1)}$$

$$+\frac{x^{2\nu+2}}{2(\rho^{2\nu+2}-1)} + \frac{x^{2\nu}(\nu+1)}{(\rho^{2\nu+2}-1)^2}\left\{\frac{1-\rho^{2\nu+4}}{2\nu+4} + \frac{\rho^2(\rho^{2\nu}-1)}{2\nu}\right\} +$$

$$+\frac{2(\nu+1)x^{2\nu}\,(B-1)(1-e^{-B\lambda\tau})}{(\rho^{2\nu+2}-1)\Theta B^2\lambda}$$

$$+\sum_{n=1}^{\infty} 2F_{II}(x,\rho,\alpha)\left\{\frac{e^{s_{n_1}\tau}(s_{n_1}+\lambda)^2}{\Theta s_{n_1}\{(s_{n_1}+\lambda)^2 + (B-1)\lambda^2\}} + \frac{e^{s_{n_2}\tau}(s_{n_2}+\lambda)^2}{\Theta s_{n_2}\{(s_{n_2}+\lambda)^2+(B-1)\lambda^2\}}\right\}\Bigg]$$

In anlogy with the above derivation of U_{II} it can be shown that the inverse transform of u_{III} is given by:

$$U_{III} = L^{-1}\{u_{III}\} = 2\nu\Bigg[\frac{2(\nu+1)x^{2\nu}\tau}{(\rho^{2\nu+2}-1)\Theta B} - \frac{(\nu+1)x^{2\nu}-1}{2\nu(\rho^{2\nu+2}-1)} + \frac{x^{2\nu+2}}{2(\rho^{2\nu+2}-1)}$$

$$+\frac{x^{2\nu}(\nu+1)}{(\rho^{2\nu+2}-1)^2}\left\{\frac{1-\rho^{2\nu+4}}{2\nu+4} + \frac{\rho^2(\rho^{2\nu}-1)}{2\nu}\right\} + \frac{2(\nu+1)x^{2\nu}}{(\rho^{2\nu+2}-1)}\,\frac{(B-1)(1-e^{-B\lambda\tau})}{\Theta B^2\lambda}$$

$$+\sum_{n=1}^{\infty} 2F_{III}(x,\rho,\alpha)\left\{\frac{e^{s_{n_1}\tau}(s_{n_1}+\lambda)^2}{\Theta s_{n_1}\{s_{n_1}+\lambda)^2+(B-1)\lambda^2\}} + \frac{e^{s_{n_2}\tau}(s_{n_2}+\lambda)^2}{\Theta s_{n_2}\{(s_{n_2}+\lambda)^2+(B-1)\lambda^2\}}\right\}\Bigg]$$

where $F_{III}(x,\rho,\alpha) = \dfrac{\pi\alpha}{2}\,\dfrac{J^2_{\nu+1}(\alpha)\{J_{\nu}(\alpha x)Y_{\nu+1}(\rho\alpha)-Y_{\nu}(\alpha x)J_{\nu+1}(\rho\alpha)\}}{\{J^2_{\nu+1}(\alpha) - J^2_{\nu+1}(\rho\alpha)\}}$

Combining U_I, U_{II} and U_{III} finally gives the solution for U sought for:

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

$$Q\left[\frac{2(\nu+1)x^{2\nu}}{\rho^{2\nu+2}-1}\cdot\frac{\tau}{\Theta B} + \frac{x^{2\nu}(x^2-\rho^2)}{2(\rho^{2\nu+2}-1)} + \frac{\rho^2(\rho^{2\nu}-x^{2\nu})}{2\nu(\rho^{2\nu+2}-1)} + \frac{\rho^2(\rho^{2\nu}-1)x^{2\nu}(\nu+1)}{2\nu(\rho^{2\nu}-1)^2} + \right.$$

$$\left. + \frac{x^{2\nu}(\nu+1)(1-\rho^{2\nu+4})}{(2\nu+4)(\rho^{2\nu+2}-1)^2} + \frac{2(\nu+1)x^{2\nu}(B-1)(1-e^{-B\lambda\tau})}{(\rho^{2\nu+2}-1)\Theta B^2\lambda}\right]+$$

$$+ \{(Q-2\nu)x^{\nu}\pi\sum_{n=1}^{\infty} 2F_{II}(x,\rho,\alpha_n) + \frac{2\nu x^{\nu}}{\rho^{\nu+1}}\pi\sum_{n=1}^{\infty} 2F_{III}(x,\rho,\alpha_n)\} *$$

$$\left\{\frac{e^{s_{n_1}\tau}(s_{n_1}+\lambda)^2}{s_{n_1}\Theta\{(s_{n_1}+\lambda)^2+(B-1)\lambda^2\}} + \frac{e^{s_{n_2}\tau}(s_{n_2}+\lambda)^2}{s_{n_2}\Theta\{(s_{n_2}+\lambda)^2+(B-1)\lambda^2\}}\right\} \qquad \text{(A-16)}$$

with

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

$$F_{III}(x,\rho,\alpha_n) = \frac{J_{\nu+1}(\alpha)}{J_{\nu+1}(\rho\alpha)}\cdot F_{II}(x,\rho,\alpha_n)$$

α_n is the n-th root of $Y_{\nu+1}(\rho x)J_{\nu+1}(x)-Y_{\nu+1}(x)J_{\nu+1}(\rho x) = 0$

and $$s_{n_{1,2}} = \frac{-(B\lambda\Theta+\alpha^2_n) \pm\sqrt{(B\lambda\Theta+\alpha^2_n)^2 - 4\lambda\alpha^2_n}}{2\Theta}$$

Other solutions can be derived from (A-16) by taking the appropriate limits. The solution for instantaneous adsorption is found by taking the limit as $\lambda \to \infty$

From (A-13) it can be seen that

$$\lim_{\lambda\to\infty} s_{n_2} = -B\lambda$$

and so: $$\lim_{\lambda\to\infty} \frac{e^{s_{n_2}\tau}(s_{n_2}+\lambda)^2}{s_{n_2}\Theta\{(s_{n_2}+\lambda)^2+(B-1)\lambda^2\}} = 0$$

As $s_{n_1} \cdot s_{n_2} = \frac{\lambda\alpha_n^2}{\Theta}$ it follows that $\lim_{\lambda \to \infty} s_{n_1} = \frac{-\alpha_n^2}{B\Theta}$

and from this $\lim_{\lambda \to \infty} \frac{e^{s_{n_1}\tau}(s_{n_1}+\lambda)^2}{s_{n_1}\Theta\{(s_{n_1}+\lambda)^2+(B-1)\lambda^2\}} = \frac{1}{s_{n_1}B\Theta} = \frac{1}{\alpha_n^2}\exp\left(\frac{-\alpha_n^2\tau}{B\Theta}\right)$

Also quite simply: $\lim_{\lambda \to \infty} \frac{2(\nu+1)x^{2\nu}(B-1)(1-e^{-B\lambda\tau})}{(\rho^{2\nu}-1)\Theta B^2\lambda} = 0$

The solution for instantaneous adsorption is thus:

$$U = \left(\frac{\rho^2-1}{\rho^{2\nu+2}-1}\right)(\nu+1)x^{2\nu}$$

$$+ Q\left\{\frac{2(\nu+1)x^{2\nu}}{\rho^{2\nu+2}-1}\cdot\frac{\tau}{\Theta B} + \frac{x^{2\nu}(x^2-\rho^2)}{2(\rho^{2\nu+2}-1)} + \frac{\rho^2(\rho^{2\nu}-x^{2\nu})}{2\nu(\rho^{2\nu+2}-1)} + \frac{\rho^2(\rho^{2\nu}-1)x^{2\nu}(\nu+1)}{2\nu(\rho^{2\nu+2}-1)^2}\right.$$

$$\left. + \frac{x^{2\nu}(\nu+1)(1-\rho^{2\nu+4})}{(2\nu+4)(\rho^{2\nu+2}-1)^2}\right\}$$

$$+ (Q-2\nu)x^\nu\pi\sum_{n=1}^{\infty}\exp\left(\frac{-\alpha_n^2\tau}{B\Theta}\right)\frac{J_{\nu+1}(\alpha_n)J_{\nu+1}(\rho\alpha_n)\{J_\nu(\alpha_n x)Y_{\nu+1}(\rho\alpha_n)-Y_\nu(\alpha_n x)J_{\nu+1}(\rho\alpha_n)\}}{\alpha_n\{J^2_{\nu+1}(\alpha_n)-J^2_{\nu+1}(\rho\alpha_n)\}}$$

$$+ \frac{2\nu\pi x^\nu}{\rho^{\nu+1}}\sum_{n=1}^{\infty}\exp\left(\frac{-\alpha_n^2\tau}{B\Theta}\right)\frac{J^2_{\nu+1}(\alpha_n)\{J_\nu(\alpha_n x)Y_{\nu+1}(\rho\alpha_n)-Y_\nu(\alpha_n x)J_{\nu+1}(\rho\alpha_n)\}}{\alpha_n\{J^2_{\nu+1}(\alpha_n)-J^2_{\nu+1}(\rho\alpha_n)\}} \qquad (A\text{-}17)$$

Likewise the solution for transport by diffusion only can be derived by substituting $\nu = 0$, or where necessary taking the limit as $\nu \to 0$. The latter has to be done for those terms where ν is a factor in the denominator:

$$\lim_{\nu \to 0}\frac{\rho^2(\rho^{2\nu}-x^{2\nu})}{2\nu(^{2\nu+2}-1)} = \frac{\rho^2}{\rho^2-1}\lim_{\nu \to 0}\frac{e^{2\nu\ln\rho}-e^{2\nu\ln x}}{2\nu} =$$

$$\frac{\rho^2}{\rho^2-1}\lim_{\nu \to 0}\frac{1+2\nu\ln\rho + (2\nu\ln\rho)^2/2! + \ldots\ldots - 1-2\nu\ln x - \ldots\ldots}{2\nu}$$

$$= \frac{\rho^2}{\rho^2-1}\lim_{\nu \to 0}\ \ln\frac{\rho}{x} + 0(\nu) = \frac{\rho^2}{\rho^2-1}\ln\frac{\rho}{x}$$

and

$$\lim \frac{\rho^2(\rho^{2\nu}-1)x^{2\nu}(\nu+1)}{2\nu(\rho^{2\nu+2}-1)^2} = \frac{\rho^2}{(\rho^2-1)^2} \lim_{\nu \to 0} \frac{2\nu\ln\rho+(2\nu\ln\rho)^2/2!+\ldots\ldots}{2\nu}$$

$$= \frac{\rho^2}{(\rho^2-1)^2} \ln\rho$$

The solution for transport by diffusion only is thus given by:

$$U = 1 + Q\left[\frac{2\tau}{(\rho^2-1)\Theta B} + \frac{x^2-\rho^2}{2(\rho^2-1)} + \frac{\rho^2}{\rho^2-1}\ln\frac{\rho}{x} + \frac{\rho^2}{(\rho^2-1)^2}\ln\rho - \frac{(1+\rho^2)}{4(\rho^2-1)}\right.$$

$$\left. + \frac{2}{\rho^2-1} + \frac{(B-1)(1-e^{-B\lambda\tau})}{\Theta B^2\lambda}\right]$$

$$- Q\pi \sum_{n=1}^{\infty} \frac{\alpha_n J_1(\alpha n) J_1(\rho\alpha_n)\{J_0(\alpha_n x)Y_1(\rho\alpha_n)-Y_0(\alpha_n x)J_1(\rho\alpha_n)}{2\{J^2{}_1(\alpha_n)-J^2{}_1(\rho\alpha_n)\}} *$$

$$\left\{ \frac{e^{s_{n_1}\tau}(s_{n_1}+\lambda)^2}{s_{n_1}\Theta\{(s_{n_1}+\lambda)^2 + (B-1)\lambda^2\}} + \frac{e^{s_{n_2}\tau}(s_{n_2}+\lambda)^2}{s_{n_2}\Theta\{(s_{n_2}+\lambda)^2+(B-1)\lambda^2\}} \right\} \qquad \text{(A-18)}$$

Finally the solution for the case where transport is by diffusion only and adsorption is instantaneous can be derived either taking the limit of (A-17) when $\nu \to 0$ or of (A-18) when $\lambda \to \infty$ leading to:

$$U = 1 + Q\left[\frac{2\tau}{(\rho^2-1)\Theta B} + \frac{x^2-\rho^2}{2(\rho^2-1)} + \frac{\rho^2}{\rho^2-1}\ln\frac{\rho}{x} + \frac{\rho^2}{(\rho^2-1)^2}\ln\rho - \frac{(1+\rho^2)}{4(\rho^2-1)}\right]$$

$$+ Q\pi \sum_{n=1}^{\infty} \exp\left(\frac{-\alpha_n^2\tau}{B\Theta}\right) \frac{J_1(\alpha_n)J_1(\rho\alpha_n)\ \{J_0(\alpha_n x)Y_1(\rho\alpha_n)-Y_0(\alpha_n x)J_1(\rho\alpha_n)\}}{\alpha_n\ \{J^2{}_1(\alpha_n)-J^2{}_1(\rho\alpha_n)\}} \qquad \text{(A-19)}$$

If adsorption is instantaneous the adsorbed solute is at any distance and time proportional to the dissolved solute or in dimensionless form: $V(x,\tau) = U(x,\tau)$.

In case of non-instantaneous adsorption one could solve for v from (A-2) and (A-9) and find V as $L^{-1}\{v\}$in a similar way as U was found as $L^{-1}\{u\}$.

It is easier however to write V as:

$$V = L^{-1}\left\{\frac{\lambda}{s+\lambda}u\right\} + e^{-\lambda\tau}$$

and find $L^{-1}\left\{\frac{\lambda}{s+\lambda}u\right\}$ with the convolution theorem:

$$L^{-1}\left\{\frac{\lambda}{s+\lambda}u\right\} = \int_0^\tau U(z,x)\lambda e^{-\lambda(\tau-z)}\,dz \tag{A-20}$$

The various terms of U, as given by A-16, fall into different categories as far as the convolution integral of the RHS of A-20 is concerned:

1. Terms not being a function of τ, and represented by f(x). The convolution integral for these terms is:

$$\int_0^\tau f(x)\lambda e^{-\lambda(\tau-z)}\,dz = f(x)(1-e^{-\lambda\tau})$$

2. Terms linear in τ, denoted by $q(x)\tau$, leads to

$$\int_0^\tau \lambda q(x)\tau e^{-\lambda(\tau-z)} = \frac{q(x)e^{-\lambda\tau}}{\lambda}\left[e^{\lambda z}(\lambda z-1)\right]_0^\tau = q(x)\tau+\frac{q(x)}{\lambda}\,(e^{-\lambda\tau}-1)$$

3. For the term with the factor $(1-e^{-B\lambda\tau})$ represented by $p(x)(1-e^{-B\lambda\tau})$ the convolution integral becomes:

$$\int_0^\tau \lambda p(x)(1-e^{-B\lambda z})e^{-\lambda(\tau-z)}dz =$$

$$p(x)e^{-\lambda\tau}\left[e^{\lambda z}\;\frac{-e^{(1-B)\lambda z}}{1-B}\right]_0^\tau = p(x)\{1-\frac{e^{-B\lambda\tau}}{1-B}+\frac{Be^{\lambda\tau}}{1-B}\}$$

Finally, terms of the series remain. Assuming uniform convergence of the series, summation and integration can be interchanged, and for the n-th term the convolution integral is of the form:

$$\int_0^\tau r(x,s_{n_1})\,\lambda e^{s_{n_1}}e^{-\lambda(\tau-z)}dz = r(x,s_{n_1})\lambda\,\frac{(e^{s_{n_1}\tau}-e^{-\lambda\tau})}{(s_{n_1}+\lambda)}$$

Combination of all the above derived components of V yields the solution as given in (16) in the main text.

APPENDIX II. Definitions and some properties of Besselfunctions

The definitions and properties given below are employed in the derivations in Appendix I and selected from Abramowitz & Stegun (1970).

p1. $J_\nu(z) = (\frac{z}{2})^\nu \sum_{k=0}^{\infty} \frac{(-z^2/4)^k}{k!\Gamma(\nu+k+1)}$

p2. $Y_\nu(z) = \frac{J_\nu(z)\cos\nu\pi - J_{-\nu}(z)}{\sin\nu\pi}$

p3. $I_\nu(z) = (\frac{z}{2})^\nu \sum_{k=0}^{\infty} \frac{(z^2/4)^k}{k!\Gamma(\nu+k+1)}$

p4. $I_\nu(z) = e^{\frac{-\nu\pi i}{2}} J_\nu(ze^{\frac{\pi i}{2}})$

p5. $K_\nu(z) = \frac{\pi}{2\sin\nu\pi}\{I_{-\nu}(z) - I_\nu(z)\}$

p6. $K_\nu(ze^{\pm\frac{\pi i}{2}}) = \pm\frac{\pi}{2}e^{\mp\frac{\nu\pi i}{2}}\{-J_\nu(z) \pm iY_\nu(z)\}$

p7. $2 I_\nu(z) = zI_{\nu-1}(z) - z\, I_{\nu+1}(z)$

p8. $2\nu K_\nu(z) = z\, K_{\nu+1}(z) - z\, K_{\nu-1}(z)$

p9. $\frac{d}{dz} I_\nu(z) = I_{\nu-1}(z) - \frac{\nu}{z} I_\nu(z)$

p10. $\frac{d}{dz} K_\nu(z) = \frac{-\nu}{z} K_\nu(z) - K_{\nu-1}(z)$

p11. $\frac{d}{dz} z^\nu I_\nu(z) = z^\nu I_{\nu-1}(z)$

p12. $\frac{d}{dz}\, z^\nu K_\nu(z) = -z^\nu K_{\nu-1}(z)$

p13. $J_\nu(z)Y'_\nu(z) - Y_\nu(z)J'_\nu(z) = \frac{2}{\pi z}$

APPENDIX III. The computer program

The program shown pertains to the calculation of equation 15 and 16 in the main text. Though the program should for a great deal be self-explanatory a few remarks about its set-up and design seem warranted. In constructing the program emphasis was put on readability and ease of use rather than on efficiency of computation. Principally the program calculates the complete solution for various root densities (the variable W in line 7) and times (TIM line 8). The program is meant to be used via a terminal from which some parameter values have to be entered (line 11 through 30). During computation some subroutines are called which are not shown as they are part of a mathematical subroutine library. The subroutine ZEJNU (line 44) calculates the zeros of $Y_{\nu+1}(x)J_{\nu+1}(\rho x) - Y_{\nu+1}(\rho x)J_{\nu+1}(x)$. The subroutines BESFRJ and BESFRY (line 84-100) compute Besselfunctions of first, resp. second kind and fractional order. In calculating the series in line 83-130 (parts c and d of equation 15 and 16) it was assumed that a maximum of 50 terms would suffice to approximate the infinite summation. This number of terms was found in prelminary calculations by trial and error. If a term of the series is less than 10^{-8} of the partial sum (line 126), the summation is halted and the outcome of the series is approximated by the partial sum.

Table A III-1 shows for a specific value of x(1) and $\tau(160)$ the values of α_n, s_{1_n}, s_{2_n}, and the corresponding terms from the series in 15c and 15d. It can be seen that with increasing α_n the value of s_{n_2} tends to α_n^2/Θ, and that of s_{n_1} to $\lambda(1.44406\ E-04)$ as follows from (A-13) and (A-14) in appendix I.

TABLE A III-1. The first 50 values of α_n (ALPH), s_{n_1} (s_1), s_{n_2} (s_2), and the corresponding terms of the series of eq. 15c (TERM 1) and 15d (TERM 2).

I	ALPH	S1	S2	TERM 1	TERM 2
1	1.68582E-01	-9.57252E-05	-1.71490E-01	-3.06775E-01	2.69541E+00
2	3.11883E-01	-1.25734E-04	-4.46866E-01	-5.40375E-02	-3.79160E-01
3	4.55043E-01	-1.34990E-04	-8.86027E-01	-1.62495E-02	1.01394E-01
4	5.98569E-01	-1.38810E-04	-1.49091E+00	-6.45582E-03	-3.75163E-02
5	7.42463E-01	-1.40719E-04	-2.26277E+00	-3.04358E-03	1.68791E-02
6	8.86663E-01	-1.41801E-04	-3.20245E+00	-1.61219E-03	-8.65581E-03
7	1.03111E+00	-1.42471E-04	-4.31049E+00	-9.29548E-04	4.87540E-03
8	1.17575E+00	-1.42913E-04	-5.58728E+00	-5.71782E-04	-2.94724E-03
9	1.32043E+00	-1.43220E-04	-7.03306E+00	-3.70148E-04	1.88277E-03
10	1.46546E+00	-1.43441E-04	-8.64802E+00	-2.49750E-04	-1.25729E-03
11	1.61048E+00	-1.43606E-04	-1.04323E+01	-1.74377E-04	8.70670E-04
12	1.75558E+00	-1.43732E-04	-1.23860E+01	-1.25305E-04	-6.21521E-04
13	1.90075E+00	-1.43831E-04	-1.45091E+01	-9.22910E-05	4.55300E-04
14	2.04598E+00	-1.43909E-04	-1.68019E+01	-6.94237E-05	-3.40960E-04
15	2.19121E+00	-1.43973E-04	-1.92634E+01	-5.32157E-05	2.60380E-04
16	2.33656E+00	-1.44025E-04	-2.18958E+01	-4.14413E-05	-2.02134E-04
17	2.48191E+00	-1.44068E-04	-2.46973E+01	-3.27444E-05	1.59287E-04
18	2.62729E+00	-1.44104E-04	-2.76684E+01	-2.62070E-05	-1.27192E-04
19	2.77270E+00	-1.44135E-04	-3.08092E+01	-2.12215E-05	1.02791E-04
20	2.91813E+00	-1.44161E-04	-3.41196E+01	-1.73607E-05	-8.39457E-05
21	3.06358E+00	-1.44184E-04	-3.75998E+01	-1.43366E-05	6.92185E-05
22	3.20904E+00	-1.44203E-04	-4.12496E+01	-1.19445E-05	-5.75930E-05
23	3.35452E+00	-1.44221E-04	-4.50691E+01	-1.00286E-05	4.82982E-05
24	3.50002E+00	-1.44236E-04	-4.90583E+01	-8.48161E-06	-4.08056E-05
25	3.64553E+00	-1.44249E-04	-5.32172E+01	-7.22158E-06	3.47096E-05
26	3.79105E+00	-1.44261E-04	-5.75459E+01	-6.18518E-06	-2.97093E-05
27	3.93658E+00	-1.44271E-04	-6.20443E+01	-5.32868E-06	2.55724E-05
28	4.08211E+00	-1.44281E-04	-6.67123E+01	-4.61567E-06	-2.21357E-05
29	4.22766E+00	-1.44289E-04	-7.15502E+01	-4.01748E-06	1.92549E-05
30	4.37321E+00	-1.44297E-04	-7.65577E+01	-3.51385E-06	-1.68320E-05
31	4.51877E+00	-1.44304E-04	-8.17349E+01	-3.08533E-06	1.47718E-05
32	4.66434E+00	-1.44310E-04	-8.70819E+01	-2.72108E-06	-1.30218E-05
33	4.80991E+00	-1.44316E-04	-9.25987E+01	-2.40798E-06	1.15184E-05
34	4.95549E+00	-1.44321E-04	-9.82851E+01	-2.13909E-06	-1.02284E-05
35	5.10107E+00	-1.44326E-04	-1.04141E+02	-1.90663E-06	9.11351E-06
36	5.24666E+00	-1.44330E-04	-1.10167E+02	-1.70489E-06	-8.14665E-06
37	5.39211E+00	-1.44334E-04	-1.16357E+02	-1.52954E-06	7.30630E-06
38	5.53783E+00	-1.44338E-04	-1.22728E+02	-1.37573E-06	-6.56986E-06
39	5.68343E+00	-1.44341E-04	-1.29263E+02	-1.24084E-06	5.92421E-06
40	5.82903E+00	-1.44344E-04	-1.35968E+02	-1.12238E-06	-5.35739E-06
41	5.97463E+00	-1.44347E-04	-1.42843E+02	-1.01683E-06	4.85264E-06
42	6.12024E+00	-1.44350E-04	-1.49887E+02	-9.24198E-07	-4.40961E-06
43	6.26585E+00	-1.44353E-04	-1.57101E+02	-8.41451E-07	4.01397E-06
44	6.41146E+00	-1.44355E-04	-1.64485E+02	-7.67808E-07	-3.66198E-06
45	6.55707E+00	-1.44357E-04	-1.72038E+02	-7.02070E-07	3.34801E-06
46	6.70268E+00	-1.44359E-04	-1.79762E+02	-6.43376E-07	-3.06739E-06
47	6.84830E+00	-1.44361E-04	-1.87655E+02	-5.90639E-07	2.81545E-06
48	6.99392E+00	-1.44363E-04	-1.95717E+02	-5.43081E-07	-2.58841E-06
49	7.13954E+00	-1.44365E-05	-2.03950E+02	-5.00249E-07	2.38430E-06
50	7.28516E+00	-1.44355E-04	-2.12352E+02	-4.61668E-07	-2.20001E-06

```
      REAL U(10),W(4),TERM2(50),BJ(2),BY(2),TIM(10),DIST(10)
      REAL ALPH(50),ARG1(50,6),ARG2(50),TERM1(50),S(50,2)
      REAL JNA,ARG12(50,6),V(6),JN1A,JN1RA,JNXA
      COMMON /PAR/ RHO,DENOM,B,WC,ALAB,ORD,TNU,ORD1,P(6)
C
C **************** CONSTANTS *****************
C
      DATA PI/3.141592654/
C RO RADIUS ROOT CM, AK ADSORPTION CONSTANT
C WC WATERCONTENT , DACC DIFFUSION COEFFICIENT CM2/DAY,
C HSC = LENGTH OF ROOT CM , AAA UPTAKE RATE MG/(CM2.DAY)
      DATA RO,AK,WC,DACC,HSC,AAA/.025,100.,.25,.1,20.,
     $4.4E-3/
C W ROOT-DENSITY CM/CM3
      DATA W/.5,1.,3.,5./
      DATA TIM/1.,5.,10.,20.,50.,75.,100.,125.,150.,200./
      DATA N/50/
C
       OPEN(UNIT=1,NAME='DX1:ALP.DAT',TYPE='NEW')
C
C **************** INPUT OF PARAMETERS ********************
C
      TYPE 701
701   FORMAT(1X,'GIVE EVAP')
      ACCEPT 300,EVAP
      TYPE 301
301   FORMAT(1X,'GIVE IIW EN NIW')
      ACCEPT 300,BIW,FIW
      IIW=BIW
      NIW=FIW
      TYPE 202
202   FORMAT(1X,'GIVE CI')
      ACCEPT 300,CI
      TYPE 203
203   FORMAT(1X,'GIVE IT,NT')
      ACCEPT 300,BIT,FIT
      IT=BIT
      NIT=FIT
2     TYPE 201
201   FORMAT(1H0,'GIVE HALFT')
      ACCEPT 300,HALFT
300   FORMAT(F10.0)
C
C EVAP = EVAPORATION RATE CM/DAY , CI INITIAL CONCENTRATION MG/ML
C HALFT HALFTIME ADSORPTION REACTION DAY
      DO 700 IW=IIW,NIW
      RDENS=W(IW)
C
C ******************* CALCULATION DIMENSIONLESS GROUPS ************
C
      ETA=HSC/RO
       B=AK/WC+1.
      TNU=-EVAP/(2.*PI*ETA*RO*RDENS*DACC)
      ORD=TNU/2.
```

```
FORTRAN IV      V02.5             THU 25-JUN-81 12:40:45
MAS,MAS=MAS.RED

0037            ORD1=ORD+1.
0038            R1=1./SQRT(PI*RDENS)
0039            RHO=R1/RO
0040            ALAB=ALOG(2.)/HALFT*RO*RO/DACC
0041            PHI=DACC*CI/(AAA*RO)
0042            Q=-RHO*RHO/(2.*ETA*PHI)
          C
          C **************** CALCULATION ZERO'S OF CROSSPRODUCT OF BESSEL-
          C FUNCTIONS, AND COEFFICIENTS OF TAU IN EXPONENT
          C
0043            DO 10 I=1,N
0044            CALL ZEJYNU(A,I,RHO,ORD,20.,.1,E-5,7)
0045             ALPH(I)=A
0046            A2=B*ALAB*WC + ALPH(I)**2
0047             DISC=A2**2-4.*WC*ALAB*ALPH(I)**2
0048             S(I,2)=(-A2-SQRT(DISC))/(2.*WC)
0049             S(I,1)=-2.*ALAB*ALPH(I)**2/(A2+SQRT(DISC))
0050      10    CONTINUE
          C
0051            WRITE(1,400) (I,ALPH(I),S(I,1),S(I,2),I=1,N)
0052      400   FORMAT(1H0,1X,'I',11X,'ALPH',13X,'S1',
               *13X,'S2'/(1X,I2,1P3E15.5))
          C
0053            WRITE(1,500)AK,WC,DACC,RO,RDENS,ALAB,RHO,TNU,PHI,Q
0054      500   FORMAT(1H0,'PARAMETERS'
               1/1X,'AK     ='1PE15.5,1X,'ML/CM3'
               2/1X,'WC     ='1PE15.5,1X,'ML/CM3'
               3/1X,'DACC   ='1PE15.5,1X,'CM2/DAY'
               4/1X,'RO     ='1PE15.5,1X,'CM'
               5/1X,'RDENS  ='1PE15.5,1X,'CM-2'
               6/1X,'ALAB   ='1PE15.5/1X,'RHO    ='1PE15.5
               7/1X,'TNU    ='1PE15.5
               8/1X,'PHI    ='1PE15.5/1X,'Q      ='1PE15.5)
          C
          C
          C **************** CALCULATION TAUC ********************
          C
0055            DELX=(RHO-1.)/5.
0056            SUMR=STRA(1.,0.)
0057            P1=2.*ORD1/(RHO**(TNU+2.)-1.)
0058            P1=P1/(B*WC)
0059            FST=(RHO*RHO-1.)
               */(RHO**(TNU+2.)-1.)*ORD1*1.**TNU
0060            TAUC=-1./P1*(FST/Q+SUMR)
0061            DO 80 J=1,6
0062            X=1.+DELX*(J-1.)
0063            FST=(RHO*RHO-1.)
               */(RHO**(TNU+2.)-1.)*ORD1*X**TNU
0064            U(J)=STRA(X,TAUC)*Q+FST
0065      80    CONTINUE
0066            WRITE(1,800)
0067      800   FORMAT(1H0,'TAUC, U(TAUC) IN CASE OF STEADY-RATE')
0068            WRITE(1,600)TAUC,(J,DIST(J),U(J),J=1,6)
0069            OTAU=-1.
```

```
C
C *************** CALCULATION COMPLETE SOLUTION ***************
C
      DO 70 ITIM=IT,NIT
      TAU=DACC*TIM(ITIM)/(RO*RO)
      EXPL=EXP(-ALAB*TAU)
C
       DO 30 J=1,6
      X=1.+DELX*(J-1)
      IX=X
      X=IX
      XTNU=X**TNU
      DIST(J)=X
C
      OTERM1=1.
      SUM1=0.
      SUM2=0.
      VSUM1=0.
      VSUM2=0.
C
C ***************** CALCULATION OF SERIES ***************
C
        DO 40 I=1,N
      IF(OTAU.EQ.TAU)GO TO 41
      A=ALPH(I)
      RA=RHO*A
      AX=A*X
      CALL BESFRJ(A,ORD,7,BJ)
      JN1A=BJ(2)
      CALL BESFRJ(AX,ORD,7,BJ)
      JNXA=BJ(1)
      CALL BESFRJ(RA,ORD1,7,BJ)
      JN1RA=BJ(1)
      CALL BESFRY(AX,ORD,7,BY)
      YNXA=BY(1)
      CALL BESFRY(RA,ORD1,7,BY)
      YN1RA=BY(1)
      ARG1(I,J)=-PI*A*JN1A*JN1RA*(JNXA*YN1RA-YNXA*JN1RA)/
     $(JN1A*JN1A-JN1RA*JN1RA)
      ARG12(I,J)=JN1A*ARG1(I,J)/JN1RA
 41   CONTINUE
      E1=S(I,1)*TAU
      E2=S(I,2)*TAU
      FAC1=(S(I,1)+ALAB)**2/
     1(WC*S(I,1)*((S(I,1)+ALAB)**2+(B-1.)*ALAB**2))
      FAC2=(S(I,2)+ALAB)**2/
     2(WC*S(I,2)*((S(I,2)+ALAB)**2+(B-1.)*ALAB**2))
      EX1=EXP(E1)*FAC1
      IF(E2.LE.-87.4) GO TO 25
      EX2=EXP(E2)*FAC2
      GO TO 26
 25   EX2=0.
 26   ARG2(I)=EX1+EX2
      TERM1(I)=ARG1(I,J)*ARG2(I)
```

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FORTRAN IV      V02.5            THU 25-JUN-81 12:40:45
MAS,MAS=MAS.RED

0115          VTERM1=ARG1(I,J)*((EXP(E1)-EXPL)*FAC1/(S(I,1)+ALAB)+
             $ (EX2/FAC2-EXPL)*FAC2/(S(I,2)+ALAB))*ALAB
0116          TERM2(I)=ARG12(I,J)*ARG2(I)
0117          VTERM2=TERM2(I)/TERM1(I)*VTERM1
0118          IF(ABS(TERM1(I)).LE.0.29E-28)GO TO 50
0120          IF(ABS(TERM1(I)/OTERM1).LE.1.E-8)GO TO 50
0122          OTERM1=TERM1(I)
0123          SUM1=SUM1+TERM1(I)
0124          SUM2=SUM2+TERM2(I)
0125          VSUM1=VSUM1+VTERM1
0126          VSUM2=VSUM2+VTERM2
0127          IF(ABS(TERM1(I)/SUM1).LE.1.E-8) GO TO 50
0129   40     CONTINUE
0130   50     CONTINUE
       C
       C ******************* STEADY-STATE PART ****************
       C
0131          FST=(RHO*RHO-1.)
             $/(RHO**(TNU+2.)-1.)*ORD1*X**TNU
       C
       C ******************* STEADY-RATE PART *****************
       C
0132          USTR=STRA(X,TAU)*Q
0133          VSTRA=0.
0134          P(1)=P(1) + P(1)/(ALAB*TAU)*(EXP(-ALAB*TAU)-1.)
0135          EXPLO=1.-EXP(-B*ALAB*TAU)/(1.-B)+B*EXPL/(1.-B)
0136          P(6)=2.*ORD1*XTNU*(B-1.)*EXPLO/
             $(DENOM*WC*B*B*ALAB)
0137          DO 89 I=2,5
0138          P(I)=P(I)*(1.-EXPL)
0139   89     CONTINUE
0140          DO 90 I=1,6
0141          VSTRA=VSTRA+P(I)
0142   90     CONTINUE
0143          VSTR=VSTRA*Q
0144          VSUM1=VSUM1*(Q-TNU)*X**ORD
0145          VSUM2=VSUM2*TNU*X**ORD/(RHO*ORD1)
0146          SUM1=SUM1*(Q-TNU)*X**ORD
0147          SUM2=SUM2*TNU*X**ORD/(RHO**ORD1)
       C
       C ******************* TOTAL SOLUTION ********************
       C
0148          U(J)=USTR + SUM1 + SUM2 + FST
0149          V(J)=VSTR+VSUM1+VSUM2+FST*(1.-EXPL) + EXPL
0150          WRITE(1,402) X,SUM1,SUM2,USTR,FST
0151          WRITE(1,402) X,VSUM1,VSUM2,VSTR,FST
0152   402    FORMAT(1H0,'X='1PE15.5,2X,'SUM1='1PE15.5,
             12X,'SUM2='1PE15.5,2X,'USTR='1PE15.5,2X,'FST ='1PE15.5)
0153   30     CONTINUE
0154          OTAU=TAU
0155          WRITE(1,601)TAU,(J,DIST(J),U(J),V(J),J=1,6)
0156   600     FORMAT(1H0,'TAU ='1PE15.5/
             11X,'J',11X,'DIST',14X,'U'/(1X,I2,1P2E15.5))
0157   601     FORMAT(1H0,'TAU ='1PE15.5/
```

```
                  11X,'J',11X,'DIST',14X,'U',14X,'V'/(1X,I2,1P3E15.5))
0158      .       IF(U(1).LT.0..OR.TAU.GT.ABS(TAUC))GO TO 700
0160    70        CONTINUE
        C
0161    700       CONTINUE
0162              CLOSE(UNIT=1,DISP='PRINT')
0163              STOP
0164              END
```

```
FORTRAN IV DIAGNOSTICS FOR PROGRAM UNIT .MAIN.

IN LINE 0043, WARNING:  POSSIBLE MODIFICATION OF INDEX 'I'
```

FORTRAN IV STORAGE MAP FOR PROGRAM UNIT .MAIN.

LOCAL VARIABLES, .PSECT $DATA, SIZE = 010042 (2065. WORDS)

NAME	TYPE	OFFSET	NAME	TYPE	OFFSET	NAME	TYPE	OFFSET
A	R*4	007524	AAA	R*4	007324	AK	R*4	007310
AX	R*4	007646	A2	R*4	007530	BIT	R*4	007454
BIW	R*4	007434	CI	R*4	007450	DACC	R*4	007314
DELX	R*4	007540	DISC	R*4	007534	ETA	R*4	007502
EVAP	R*4	007430	EXPL	R*4	007604	EXPLD	R*4	007732
EX1	R*4	007702	EX2	R*4	007706	E1	R*4	007662
E2	R*4	007666	FAC1	R*4	007672	FAC2	R*4	007676
FIT	R*4	007460	FIW	R*4	007440	FST	R*4	007554
HALFT	R*4	007470	HSC	R*4	007320	I	I*2	007522
IIW	I*2	007444	IT	I*2	007464	ITIM	I*2	007576
IW	I*2	007474	IX	I*2	007610	J	I*2	007564
JNA	R*4	007410	JNXA	R*4	007424	JN1A	R*4	007414
JN1RA	R*4	007420	N	I*2	007330	NIT	I*2	007466
NIW	I*2	007446	OTAU	R*4	007572	OTERM1	R*4	007616
PHI	R*4	007512	PI	R*4	007300	P1	R*4	007550
Q	R*4	007516	RA	R*4	007642	RDENS	R*4	007476
RO	R*4	007304	R1	R*4	007506	SUMR	R*4	007544
SUM1	R*4	007622	SUM2	R*4	007626	TAU	R*4	007600
TAUC	R*4	007560	USTR	R*4	007722	VSTR	R*4	007736
VSTRA	R*4	007726	VSUM1	R*4	007632	VSUM2	R*4	007636
VTERM1	R*4	007712	VTERM2	R*4	007716	X	R*4	007566
XTNU	R*4	007612	YNXA	R*4	007652	YN1RA	R*4	007656

COMMON BLOCK /PAR /, SIZE = 000070 (28. WORDS)

NAME	TYPE	OFFSET	NAME	TYPE	OFFSET	NAME	TYPE	OFFSET
RHO	R*4	000000	DENOM	R*4	000004	B	R*4	000010
WC	R*4	000014	ALAB	R*4	000020	ORD	R*4	000024
TNU	R*4	000030	ORD1	R*4	000034	P	R*4	000040

LOCAL AND COMMON ARRAYS:

NAME	TYPE	SECTION	OFFSET	------SIZE-----	DIMENSIONS
ALPH	R*4	$DATA	000540	000310 (100.)	(50)
ARG1	R*4 Vec	$DATA	001050	002260 (600.)	(50,6)
ARG12	R*4 Vec	$DATA	004770	002260 (600.)	(50,6)
ARG2	R*4	$DATA	003330	000310 (100.)	(50)
BJ	R*4	$DATA	000400	000010 (4.)	(2)
BY	R*4	$DATA	000410	000010 (4.)	(2)
DIST	R*4	$DATA	000470	000050 (20.)	(10)
P	R*4	PAR	000040	000030 (12.)	(6)
S	R*4 Vec	$DATA	004150	000620 (200.)	(50,2)
TERM1	R*4	$DATA	003640	000310 (100.)	(50)
TERM2	R*4	$DATA	000070	000310 (100.)	(50)
TIM	R*4	$DATA	000420	000050 (20.)	(10)
U	R*4	$DATA	000000	000050 (20.)	(10)
V	R*4	$DATA	007250	000030 (12.)	(6)
W	R*4	$DATA	000050	000020 (8.)	(4)

FORTRAN IV STORAGE MAP FOR PROGRAM UNIT .MAIN.

SUBROUTINES, FUNCTIONS, STATEMENT AND PROCESSOR-DEFINED FUNCTIONS:

NAME	TYPE	NAME	TYPE	NAME	TYPE	NAME	TYPE	NAME	TYPE
ABS	R*4	ALOG	R*4	BESFRJ	R*4	BESFRY	R*4	EXP	R*4
SQRT	R*4	STRA	R*4	ZEJYNU	R*4				

MAS,MAS=MAS.RED

```
0001            FUNCTION STRA(X,TAU)
          C FUNCTION STRA CALCULATES THE STEADY-RATE PART OF THE SOLUTION
0002            COMMON /PAR/ RHO,DENOM,B,WC,ALAB,ORD,TNU,ORD1,P(6)
          C
0003            RHO2=RHO**(TNU+2.)
0004            DENOM=1.-RHO2
0005            DENOM=-DENOM
0006            XTNU=X**TNU
0007            P(1)=2.*ORD1*XTNU*TAU/(WC*B*DENOM)
0008            P(2)=XTNU*(X*X-RHO*RHO)/(2.*DENOM)
0009            P(3)=RHO*RHO*(RHO**TNU-XTNU)/(TNU*DENOM)
0010            P(4)=RHO*RHO*(RHO**TNU-1.)/(TNU*DENOM*DENOM)*
               $XTNU*ORD1
0011            P(5)=XTNU*ORD1*(1.-RHO**(TNU+4.))/
               $(DENOM*DENOM*(TNU+4.))
0012            IF(ALAB.LE.0.)GO TO 2
0014            IF(ABS(B*ALAB*TAU).GT.87.)GO TO 3
0016            EXPL=EXP(-B*ALAB*TAU)
0017            GO TO 4
0018      3     EXPL=0.
0019      4     CONTINUE
0020            P(6)=2.*ORD1*XTNU*(B-1.)*(1.-EXPL)/
               $(DENOM*WC*B*B*ALAB)
0021      2     CONTINUE
          C
0022            WRITE(1,500) P
0023      500   FORMAT(1H0,'TERMEN UIT STEADY-RATE :'/
               1(1P4E15.5))
0024            STRA=0.
0025            DO 1 I=1,8
0026            STRA=STRA+P(I)
0027      1     CONTINUE
0028            RETURN
0029            END
```

```
FORTRAN IV STORAGE MAP FOR PROGRAM UNIT STRA

LOCAL VARIABLES, .PSECT $DATA, SIZE = 000060 (    24. WORDS)

NAME    TYPE  OFFSET        NAME   TYPE  OFFSET       NAME   TYPE  OFFSET
EXPL    R*4   000022        I      I*2   000026       RHO2   R*4   000012
STRA    R*4   000004 Eqv TAU    R*4 @ 000002       X      R*4 @ 000000
XTNU    R*4   000016

COMMON BLOCK /PAR   /, SIZE = 000070 (    28. WORDS)

NAME    TYPE  OFFSET        NAME   TYPE  OFFSET       NAME   TYPE  OFFSET
RHO     R*4   000000        DENOM  R*4   000004       B      R*4   000010
WC      R*4   000014        ALAB   R*4   000020       ORD    R*4   000024
TNU     R*4   000030        ORD1   R*4   000034       P      R*4   000040

LOCAL AND COMMON ARRAYS:

NAME      TYPE    SECTION OFFSET  ------SIZE----- DIMENSIONS
P         R*4     PAR     000040  000030 (    12.) (6)

SUBROUTINES, FUNCTIONS, STATEMENT AND PROCESSOR-DEFINED FUNCTIONS:

NAME    TYPE    NAME    TYPE    NAME    TYPE    NAME    TYPE    NAME    TYPE
ABS     R*4     EXP     R*4
```