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

door

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1981
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ACKNOWLEDGMENT

Thanks are due to Mr. M. van Noordwijk for various critical remarks and comments.
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 \( W \text{ cm cm}^{-3} \), and suppose all roots have the same length \( h \text{ cm} \) and radius \( R_0 \text{ cm} \) (fig. 1). To each root thus a cylinder of soil can be assigned of height \( h \) and radius \( R_1 \), the latter given by:

\[
R_1 = \frac{1}{\sqrt{\pi W}} \text{ cm}
\]  

(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 \( E \text{ ml/(cm}^2\text{day)} \) 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 \((R_0 < r < R_1)\) is \( E/W \text{ ml day}^{-1} \). So the flux of water at distance \( r \) is given by:
\[ v = \frac{-E}{2\pi rhw} \text{ cm day}^{-1} \]  

(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 \( \text{ cm}^2\text{day}^{-1} \)
- \( C \) = concentration of the solute in the soil solution \( \text{ mg ml}^{-1} \)
- \( r \) = radial distance from the root midpoint \( \text{ cm} \)

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 \( \text{ mg cm}^{-3} \)
- \( t \) = time \( \text{ day} \)

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 > 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:

\[ \frac{\delta C_T}{\delta t} = D \frac{\delta}{\delta r} \frac{\delta C}{\delta r} + \frac{\delta C}{\delta r} \]

(3)

The bulk density \( C_T \) consists of two components:
\[ C_T = C_A + \Theta C \]  

(4)

where \( C_A \) = the bulk density of adsorbed solute \( \text{mg cm}^{-3} \)

\( \Theta \) = the water content \( \text{ml cm}^{-3} \)

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

\[ \frac{\partial C_A}{\partial t} + \Theta \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial r^2} r + \frac{\partial C}{\partial r} - \frac{\partial C}{\partial r} \]  

(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:

\[ \frac{\partial C_A}{\partial t} = k(KC - C_A) \]  

(6)

with

\( k \) = adsorption rate constant \( \text{day}^{-1} \)

\( K \) = adsorption coefficient \( \text{ml cm}^{-3} \)

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:

\[ r = R_1 : -2\pi h R_1 \frac{\partial C}{\partial r} + 2\pi h R_1 v C = 0 \]  

(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 \( A \text{ mg cm}^{-2}\text{day}^{-1} \), then each root has to take up \( A/W \text{ mg day}^{-1} \) in order to satisfy the demand. The second boundary condition accordingly can be formulated as:
\[ r = R_0 : -2\pi rhR_0 \frac{\delta C}{\delta t} + 2\pi rhR_0 v C = -A/W \]  

(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 \((C_{Rs})\). Line I represents the Michaelis-Menten relation found in short-term physiological 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 \(C_i\) is reached. In the calculations the broken line IV was used as the boundary instead of line I.
The limiting concentration is that concentration, when potential uptake equals plant demand, or

\[ 2\pi R_0 hm C_1 = \pi R_1^2 A \]

so that \( C_1 \) can be found as:

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

where \( m = \) root absorbing power \( \text{cm day}^{-1} \)

Initially the soil around the root is assumed to have a uniform solute bulk density, with equilibrium between adsorbed and solved solute:

\[ t = 0 : C = C_i \quad C_A = C_{A_1} = K.C_i \quad (9) \]

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

- dimensionless time \( \tau = D t/R_0^2 \)
- concentration \( U = C/C_i \)
- bulk density of adsorbed solute \( V = C_A/C_{A_1} = C_A/KC_i \)
- 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 \( B = (K+\phi)/\phi \)
- bulk density of solute \( T = (KV+\omega U)/\omega B \)

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:

\[
\begin{align*}
\frac{5V}{5t} + \frac{\delta U}{\delta t} &= \delta^2 U + \frac{1-2V}{x} \frac{\delta U}{\delta x} \\
\frac{\delta V}{\delta t} &= \lambda (U-V) \\
x = \rho: - \frac{\delta U}{\delta x} + \frac{2V}{\rho} &= 0 \\
x = 1: - \frac{\delta U}{\delta x} + 2V &= \frac{-\rho^2}{2\eta} = Q \\
\tau = 0 & \quad U = V = 1
\end{align*}
\]

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

\[
\begin{align*}
U &= \left\{ \frac{-\rho^2-1}{\rho^{2V+2}-1} \right\} (v+1)x^{2V} + \\
Q &= \frac{2(v+1)x^{2V}}{\rho^{2v+2}-1} + \frac{x^{2V}(x^2-\rho^2)}{\Theta B} + \frac{\rho^2(\rho^{2V}-x^2V)}{2(\rho^{2V+2}-1)} + \frac{\rho^2(\rho^{2V+1})x^{2V}}{2V(\rho^{2V+2}-1)^2} + \\
&\quad + \frac{x^{2V}(v+1)(1-\rho^{2V+1}x)}{(2v+4)(\rho^{2V+2}-1)^2} + \frac{2(v+1)x^{2V}(0-1-B\lambda T)}{(\rho^{2V+2}-1)\Theta B^2\lambda} + \\
&\quad + (Q-2V)x^{2V} \prod_{n=1}^{\infty} 2F_v(x, \alpha_n) G(s_{n_1}, s_{n_2}, \tau) + \\
&\quad + \frac{2vx^{2V}}{\rho^{2V+2}} + \prod_{n=1}^{\infty} \frac{2J_{\psi n}^2(\alpha)}{J_{\psi n}^2(\alpha)F_v(x, \alpha_n)G(s_{n_1}, s_{n_2}, \tau)}
\end{align*}
\]

with

\[
F_v(x, \alpha_n) = \frac{\alpha_n J_{\psi n}^2(\alpha)G(s_{n_1}, s_{n_2}, \tau)}{2\{J_{\psi n}^2(\alpha)-J_{\psi n}^2(\alpha)\}}
\]
\[-(B\lambda\theta+\alpha^2_n) \pm \sqrt{(B\lambda\theta+\alpha^2_n)^2 - 4\lambda\alpha^2_n}\]

\[s_{n_1', n_2} = \frac{s_{n_1} \tan^{-1} (s_{n_1}+\lambda)^2}{2\theta} + \frac{s_{n_2} \tan^{-1} (s_{n_2}+\lambda)^2}{2\theta}
\]

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

and \(\alpha_n\) is the \(n\)-th root of:

\[Y_{\nu+1}(\lambda \alpha)J_{\nu+1}(x) - Y_{\nu+1}(x)J_{\nu+1}(\lambda \alpha) = 0\]

\(J_{\nu}, Y_{\nu}\) are Bessel functions of first and second kind, respectively, and order \(\nu\).

The bulk density of adsorbed solute is given by:

\[v = \left(\frac{\rho^2-1}{\rho^2 v^2+2-1}\right) (v+1) x^2v (1-e^{-\lambda \tau}) + \frac{2Q(\nu+1)x^2v \tau}{(\rho^2 v^2+2-1) \Theta B} + \frac{Q(1-e^{-\lambda \tau})}{(\rho^2 v^2+2-1) \lambda} \left[\frac{-2(v+1)x^2v}{2v(\rho^2 v^2+2-1)\lambda} + \frac{x^2v}{2v(\rho^2 v^2+2-1)} + \frac{\rho^2(\rho^2 v^2-x^2v)}{2v(\rho^2 v^2+2-1)} \right] + \frac{2Q(\nu+1)x^2v}{(\rho^2 v^2+2-1) \Theta B^2 \lambda} \left[\frac{1-e^{-\lambda \tau}}{1-B} + \frac{B e^{-\lambda \tau}}{1-B} \right] + e^{-\lambda \tau} + (Q-2) y x \sum_{p=2}^{\infty} \sum_{n=0}^{\infty} 2F(\nu, \alpha_n) H(s_{n_1}, s_{n_2}, \tau) \]

\[+ \frac{2 x v}{p \nu+1} \sum_{n=0}^{\infty} \frac{2J_{\nu+1}(\lambda \alpha)}{J_{\nu+1}(\lambda \alpha)} F_{\nu}(x, \alpha_n) H(s_{n_1}, s_{n_2}, \tau)\]

with

\[H(s_{n_1}, s_{n_2}, \tau) = \frac{s_{n_1} \tan^{-1} (s_{n_1}+\lambda)^2}{s_{n_1} \Theta((s_{n_1}+\lambda)^2 + (B-1)\lambda^2)} + \frac{s_{n_2} \tan^{-1} (s_{n_2}+\lambda)^2}{s_{n_2} \Theta((s_{n_2}+\lambda)^2 + (B-1)\lambda^2)}\]
As is shown in Appendix I other solutions can be derived from (15) or (16). When transport is by diffusion only:

\[
U = 1 + \left\{ Q \frac{2}{\rho^2 - 1} \frac{\tau}{\Theta B} + \frac{x^2 - \rho^2}{2(\rho^2 - 1)} + \frac{\rho^2}{\rho^2 - 1} \ln \left( \frac{\rho}{x} \right) + \frac{\rho^2}{(\rho^2 - 1)^2} 1\ln \rho - \frac{(1+\rho^2)}{4(\rho^2 - 1)} \right. \\
+ \left. \frac{2}{\rho^2 - 1} \frac{(B-1)\left(1-e^{-B\lambda T}\right)}{\Theta B^2 \lambda} \right\} \] (17a)

\[
+ Q \pi \sum_{n=1}^{\infty} F \left( x, \alpha_n \right) G \left( s_{n_1}, s_{n_2}, \tau \right) \] (17b)

where \( \alpha_n \) now is the \( n \)-th root of:

\[
Y_1(\rho x) J_1(x) - Y_1(x) J_1(\rho x) = 0 
\]

\[
V = 1 + \left\{ \frac{2Q}{(\rho^2 - 1)} \frac{\tau}{\Theta B} + \frac{Q \left(1-e^{-\lambda T}\right)}{(\rho^2 - 1)\Theta B^2 \lambda} \left\{1 - \frac{e^{-B\lambda T}}{(1-B)} \right. \right. \\
+ \left. \frac{B e^{-\lambda T}}{(1-B)} \right\} \right. \\
+ \left. Q \pi \sum_{n=1}^{\infty} F \left( x, \alpha_n \right) H \left( s_{n_1}, s_{n_2}, \tau \right) \right\} \] (18)

The solution when adsorption is instantaneous is given by:

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

\[
+ Q \left[ \frac{2(v+1)x^{2v}}{\nu^2 v^2 + 2 - 1} \frac{\tau}{\Theta B} + \frac{x^{2v}(x^2 - \rho^2)}{2(\rho^2 \nu^2 + 2 - 1)} + \frac{\rho^2 (\rho^2 v^2 - x^2 \nu)}{2v(\rho^2 v^2 + 1)} \right. \\
+ \left. \frac{\rho^2 (\rho^2 v^2 - 1)x^2 \nu}{2v(\rho^2 v^2 + 2 - 1)} \right] \] (19a)

\[
\left. + \frac{x^{2v}(v+1)(1-\rho^{2v+4})}{(2v+4)(\rho^2 \nu^2 + 2 - 1)^2} \right] \\
+ \left( Q-2v \right)x^v \sum_{n=1}^{\infty} \frac{-\alpha_n^{2v}}{\Theta B} - \frac{2e^{2v}}{\Theta B} F \left( x, \alpha_n \right) \] (19b)

\[
+ (Q-2v)x^v \sum_{n=1}^{\infty} \frac{-\alpha_n^{2v}}{\Theta B} - \frac{2e^{2v}}{\Theta B} F \left( x, \alpha_n \right) \] (19c)
Finally when transport is simply by diffusion and adsorption instantaneous:

\[
U = 1 + \sum_{n=1}^{\infty} \frac{-\alpha^2}{\Theta B} \frac{J_{\nu+1}(\alpha)}{\alpha_n^2 J_{\nu+1}(\alpha_n)} + P
\]

(19d)

\[
\sum_{n=1}^{\infty} \frac{2\nu x^\nu}{\rho^\nu+1} \prod_{n=1}^{\infty} -2 \exp\left(-\frac{\alpha^2}{\Theta B} \frac{J_{\nu+1}(\alpha)}{\alpha_n^2 J_{\nu+1}(\alpha_n)}\right) (\alpha_n)\]

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:

\[ \frac{\delta U}{\delta x} = \frac{2v(\rho^2-1)}{\rho^{2v+2}-1} (v+1)x^{2v-1} \]

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:

\[ \frac{\delta U}{\delta x} = \frac{-2v}{x} \]

When Q ≠ 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_{n1} and s_{n2}, and of course -a_n^2 are negative), eventually thus only part a and b remain (the factor (1-e^{-BlT}) 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:

\[ \frac{\delta U}{\delta t} = \frac{2Q}{(\rho^2-1)B^2} \]

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 \( \frac{\delta U}{\delta t} \) will eventually become independent of time but will nevertheless stay a function of distance:
The contribution of mass flow to transport is governed by the parameter \( v \), the value of which both in absolute sense and in relation to the value of \( Q \) is important. Normally the value of \( v \) 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\(^{-1}\), \( v \) will assume the value:

\[
v = -\frac{0.5}{(4 \pi 20 \cdot 0.1 \cdot 1)} = -0.02
\]

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 2\( v \) is of the same order as or greater than \( Q \).

From the definitions of \( Q \) and \( v \) it follows:

\[
\frac{Q}{2v} = \frac{\rho^2}{2\eta \phi} \cdot \frac{2\eta \phi}{\rho^2} = \frac{D}{ER} = \frac{AR_a}{DG_i} = \frac{A}{BG_i}
\]

For a nutrient like phosphate the average uptake is \( 4-5 \times 10^{-3} \) 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% \( \text{P}_2\text{O}_5 \)), 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 \( Q/2v \) according will be of the order:

\[
Q/2v = 10 - 15
\]

In the coefficient \((Q-2v)\) of the infinite series in eq 15c and 19c consequently \( 2v \) 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 \( 3 \times 10^{-2} \) 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 \(Q/2v\) assumes the value: 0.075. In this case \(Q\) is of the same order or even smaller than \(2v\), 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.**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Symbol</th>
<th>Dimension</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transpiration</td>
<td>(E)</td>
<td>cm day(^{-1})</td>
<td>0 - 1</td>
</tr>
<tr>
<td>Adsorption constant</td>
<td>(K)</td>
<td>ml cm(^{-3})</td>
<td>0 (nitrate)</td>
</tr>
<tr>
<td>Water content</td>
<td>(\Theta)</td>
<td>ml cm(^{-3})</td>
<td>0.25</td>
</tr>
<tr>
<td>Diffusion coefficient</td>
<td>(D)</td>
<td>cm(^2) day(^{-1})</td>
<td>0.1</td>
</tr>
<tr>
<td>Root density</td>
<td>(W)</td>
<td>cm(^{-2})</td>
<td>0.5 - 5</td>
</tr>
<tr>
<td>Half time adsorption rate</td>
<td>(t_{0.5})</td>
<td>day</td>
<td>0 - 30</td>
</tr>
<tr>
<td>Initial concentration</td>
<td>(c_i)</td>
<td>mg ml(^{-1})</td>
<td>(10^{-3}) (P) - 0.8 (N)</td>
</tr>
<tr>
<td>Uptake rate</td>
<td>(A)</td>
<td>mg cm(^{-2}) day(^{-1})</td>
<td>(4.4 \times 10^{-3}) (P) - 3x10(^{-2}) (N)</td>
</tr>
<tr>
<td>Root radius</td>
<td>(R_o)</td>
<td>cm</td>
<td>0.025</td>
</tr>
<tr>
<td>Plow layer (root length)</td>
<td>(h)</td>
<td>cm</td>
<td>20</td>
</tr>
<tr>
<td>Root absorbing power</td>
<td>(m)</td>
<td>cm day(^{-1})</td>
<td>0.043 - 0.43 (nitrate)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>6.5 - 56 (phosphate)</td>
</tr>
</tbody>
</table>

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
around the root with time for nitrate, when transpiration is high
($E = 1\ \text{cm day}^{-1}$, fig. 3a) and when it is absent (fig. 3b). When mass flow
is occurring 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. More­
over 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
$\tau = 16000$ 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 $\tau$ 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$^{-1}$. Transpiration 1 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 and d) play a less prominent role as time proceeds. (For $\tau = 3200$ 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 $\tau_c$ - uptake of the root is completely in accordance with the demand of the plant. If it may be assumed that when $\tau$ equals $\tau_c$, the series part of (19) and (20) can be neglected, it is easy to make $\tau_c$ explicit:

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

$$- \frac{\Theta B}{2(v+1)} \left\{ \frac{1-\rho^2}{2} + \frac{\rho^2(\rho^2 v - 1)}{2v} + \frac{\rho^2(\rho^2 v - 1)}{2v(\rho^2 v^2 - 1)} + \frac{(1-\rho^2 v^2)}{(2v+1)(\rho^2 v + 2 - 1)} \right\}$$

(21)

or when transport is by diffusion only:

$$\tau_c = \frac{\Theta B(\rho^2 - 1)}{2Q} (U_1 - 1) - \frac{\Theta B}{2} \left\{ \frac{1-\rho^2}{2} + \rho^2 1n\rho + \frac{\rho^2 1n\rho}{\rho^2 - 1} \right\}$$

(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 $\tau_c$ 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 $C_i$ is zero the maximum period of unconstrained uptake is given by:

$$t_{\text{max}} = \frac{R_0}{\pi R^2 A} \frac{2\pi rh(K+\Theta)C_i}{R_1} = \frac{h(R_i^2 - R_0^2)}{R_1^2 A} (\Theta + K)C_i$$
or in dimensionless form:

\[
\tau_{\text{max}} = \frac{D t_{\text{max}}}{R_0^2} = \Theta B \phi r (\rho^2 - 1) / \rho^2
\]  

(23)

The realized fractional depletion \( F_d \) is given by:

\[
F_d = \frac{\tau_c}{\tau_{\text{max}}}
\]  

(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 $\tau_c$) 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 $U_1, \tau = 0$ as function of root density ($W$).]

If $U_1$ is greater than zero it would seem obvious to define $\tau_{\text{max}}$ as:

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

(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 $\tau_c$ is approximately 8000 while $\tau_{\text{max}}$ calculated according to (25) amounts to 5300. To overcome this difficulty $\tau_{\text{max}}$ was defined as in (24) even when $U_1 > 0$. 
As was explained earlier (section 2) $C_1$ and so $U_1$ is in fact a function of root-density:

$$U_1 = C_1/C_i = \frac{\mu^2}{2 \eta \mu}, \text{ where } \mu = \frac{mC_i}{A}$$

Nye and Tinker (1977) give values of $m$ ($\alpha$ in their notation) ranging from $2.5 \times 10^{-2} - 2 \text{ cm day}^{-1}$ (for nitrate) and from $6.5-56 \text{ cm day}^{-1}$ (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 ($F_\phi$) of nitrate as function of root-density and root absorbing power.

**Fig. 8b.** As fig. 8a for phosphate.
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 $t_1 = 0$ and $t_1 = 1$ 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 ($t_1 = 30$ days). In the beginning ($t = 1$, or $\tau = 160$) 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 \( \tau \), for finite adsorption rate
initially the term with factor \((1-e^{-B\lambda T})\) (see eq. 17b) is of some importance, very soon this factor approximates unity. Thus from \(t = 1\) \((\tau = 160)\) 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 \(T_x\) (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 \(y = T_x\), 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 \(\tau_c\) can be given as explicit function of \(\rho\) and the other parameters, if at least the parts \(c\) and \(d\) of equation (15) and (17) can be neglected:

\[
\tau_c = \frac{-(B-1)}{B_1} + \frac{\Theta B (\rho^{2V+2} - 1)}{2(V+1)Q} U_1 - \frac{\Theta B (\rho^{2} - 1)}{2Q} + \\
- \frac{\Theta B}{2(V+1)} \left\{ \frac{1-\rho^2}{2} + \frac{\rho^2(\rho^{2V} - 1)}{2V} + \frac{\rho^2(\rho^{2V} - 1)}{2V(\rho^{2V+2} - 1)} + \frac{1-\rho^{2V+4}}{(2V+4)(\rho^{2V+2} - 1)} \right\} \tag{26}
\]

Fig. 12. Contribution of the three terms of equation (17) to the concentration \(U\).
Compared with (21) and (22), (26) and (27) show that, since $B \gg 1$, $
abla_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 $U(1, \tau)$ becomes zero, rendering a calculation of $\tau_c$ with equation (27) incorrect. In fig. 15 the fractional depletion $F_d$ is plotted as function of root density and root absorbing power for $t_1 = 30$ 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 $\tau_c$ (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 $1/(\lambda \tau_{\text{max}})$ 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 $2v$ will not exceed 0.1, so choosing - for computational convenience - a value of $-0.5$ for $2v$ 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.
5. LITERATURE


Noordwijk, M. van, Raats, P.A.C., de Willigen, P. Transport models for calculation of root densities necessary for good crop growth (in prep.).
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 \( \tau \), the Laplace parameter being denoted by \( s \), then (10)-(13) with initial condition (14) transform into:

\[
K(sv-1) + \theta(su-1) = \frac{d^2u}{dx^2} + \frac{1}{x} (1-2v) \frac{du}{dx}
\]

\[
sv-1 = \lambda(u-v)
\]

for \( x = \rho \):
\[
-\frac{\delta u}{\delta x} + \frac{2v}{\rho} u = 0
\]

for \( x = 1 \):
\[
-\frac{\delta u}{\delta x} + 2vu = \frac{Q}{s}
\]

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:

\[
\beta u - \frac{\beta}{s} = \frac{d^2u}{dx^2} + \frac{1}{x} (1-2v) \frac{du}{dx}
\]

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

The solution of the homogeneous part of (A-5) is given by Abramowitz and Stegun (1970), (page 362, 9.1.52):
where $I_v$ and $K_v$ are modified Bessel functions of first resp. second kind and order $v$.

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: 

$$u = \frac{1}{s} + c_1 x^v I_v(x/\beta) + c_2 x^v K_v(x/\beta) \quad (A-6)$$

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 *)

$$\frac{du}{dx} = c_1 x^v \beta I_{v-1}(x/\beta) - c_2 x^v \beta K_{v-1}(x/\beta) \quad (A-7)$$

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

$$c_2 \beta k_{v+1}(\sqrt{\beta}) - c_1 \beta k_{v+1}(\sqrt{\beta}) = -\frac{Q-2\nu}{s} \quad (A-8)$$

$$c_2 \rho \nu k_{v+1}(\rho \sqrt{\beta}) - c_1 \rho \nu k_{v+1}(\rho \sqrt{\beta}) = -\frac{2\nu}{\rho s} \quad (A-9)$$

Solving for $c_1$ and $c_2$ results in:

*) In Appendix II some properties of Bessel functions are given relevant for the derivation treated here. These properties will from here on be referred to as p1, p2, etc.
So that eventually the solution for $u$ is given by:

$$u = \frac{1}{8} + \frac{(2v-Q)x}{s/\beta I_{v+1}(\nu/\beta) - K_{v+1}(\nu/\beta)I_{v+1}(\nu/\beta)}$$

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 straightforwardly:

$$u_I = L^{-1}\{u_I\} = 1$$

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)):
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 \( e^{St} \))

\[
I_v(x/\beta)K_{v+1}(\rho/\beta) + K_v(x/\beta)I_{v+1}(\rho/\beta) = 
\]

\[
\frac{\pi}{2\sin\pi \nu} \{ I_{-\nu}(x/\beta)I_{v+1}(\rho/\beta) - I_{\nu}(x/\beta)I_{-(v+1)}(\rho/\beta) \} 
\]

(A-11)

In deriving (A-11) use is made of the definition of \( K_v \) (p5).

If next the Bessel functions I are written as infinite series (p4) and the terms are rearranged (A-11) becomes

\[
\frac{\pi}{2\sin\pi \nu} \cdot \frac{1}{\sqrt{\nu}} \left\{ \frac{x^{1-v} \nu^+1}{\beta} - \frac{2x^v \nu^-(\nu+1)}{\Gamma(\nu+1)\Gamma(-\nu)} - \frac{\nu^2 - \nu^{(v+1)} \rho}{\Gamma(\nu+1)\Gamma(-\nu)(2+2v)} + \right. \]

\[
\left. + \frac{x^{1-v} \nu^2}{2\nu\Gamma(\nu+1)\Gamma(-\nu)} + O(\beta^2) \right\}
\]

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

Likewise the denominator can be written:

\[
K_{v+1}(\rho/\beta)I_{v+1}(\nu/\beta) - K_{v+1}(\nu/\beta)I_{v+1}(\rho/\beta) = 
\]

\[
\frac{s\nu}{2\sin\pi \nu} \left[ \frac{\nu^+1 - \nu^{(v+1)}}{\Gamma(\nu+2)\Gamma(-\nu)} + \frac{\nu^3 - \nu^{(v+1)}}{\Gamma(\nu+2)\Gamma(-\nu)(2v+4)2 - \frac{\nu^2 + \nu^{(v+1)}}{4\nu\Gamma(\nu+2)\Gamma(-\nu)} \right] \beta + O(\beta^2) \]

The integrand accordingly can be written in the form:

\[
\frac{sT}{s\beta} \left\{ \frac{a_1 + a_2 \beta + O(\beta^2)}{b_1 + b_2 \beta + O(\beta^2)} \right\}
\]

where

\[
a_1 = \frac{-2x^v \nu^{(v+1)}}{\Gamma(\nu+1)\Gamma(-\nu)}
\]

\[
s_2 = \frac{x^{v+2} - \nu^{(v+1)}}{2\nu\Gamma(\nu+1)\Gamma(-\nu)} + \frac{\rho - \nu^{(v+1)}}{2\nu\Gamma(\nu+1)\Gamma(-\nu)} - \frac{x^{v+2} - \nu^{(v+1)}}{\Gamma(\nu+1)\Gamma(-\nu)(2+2v)}
\]
or using the definition of $\beta$ given earlier:

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

(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

$$\frac{\partial \beta}{\partial s} \bigg|_{s=0} = \Theta \beta \quad \text{en} \beta \bigg|_{s=0} = 0$$

the residue at the pole $s = 0$ is given by (Churchill 1970):

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

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

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

Finally the integrand has poles for the zeros of

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

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

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

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 $\beta = -\alpha_1^2, -\alpha_2^2, \ldots$,
or when \( s \) assumes the values:

\[
\begin{align*}
    s_{n1} &= \frac{-(B\lambda\theta + \alpha_n^2) + \sqrt{(B\lambda\theta + \alpha_n^2)^2 - 4\alpha_n^2}}{2\theta} \quad (A-13) \\
    s_{n2} &= \frac{-(B\lambda\theta + \alpha_n^2) - \sqrt{(B\lambda\theta + \alpha_n^2)^2 - 4\alpha_n^2}}{2\theta} \quad (A-14)
\end{align*}
\]

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

\[
\left[ \frac{-e^{-\pi \lambda}}{sv\beta} \frac{d}{ds} \left\{ K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta}) \right\} \right] _{\beta = -\alpha_n^2} \quad (A-15)
\]

Using the properties p9 and p10 and the fact that for

\( \beta = -\alpha_n^2 : K_{\nu+1}(\rho\sqrt{\beta})I_{\nu+1}(\sqrt{\beta}) - K_{\nu+1}(\sqrt{\beta})I_{\nu+1}(\rho\sqrt{\beta}) = 0 \)

the residue for \( \beta = -\alpha_n^2 \) becomes

\[
2F_{II}(x,\rho,\alpha) = \left[ \frac{e^{s_{n1}^T (s_{n1} + \lambda)^2}}{s_{n1} \{(s_{n1} + \lambda)^2 + (\Lambda-1)^2 \lambda^2 \}} + \frac{e^{s_{n2}^T (s_{n2} + \lambda)^2}}{s_{n2} \{(s_{n2} + \lambda)^2 + (\Lambda-1)^2 \lambda^2 \}} \right]
\]

with

\[
F_{II}(x,\rho,\alpha) = \frac{K_{\nu+1}(\rho\alpha)I_{\nu}(\rho\alpha) + I_{\nu+1}(\rho\alpha)K_{\nu}(\rho\alpha)}{I_{\nu}(\rho\alpha)K_{\nu+1}(\rho\alpha) + K_{\nu}(\rho\alpha)I_{\nu+1}(\rho\alpha) - p[I_{\nu+1}(\rho\alpha)K_{\nu}(\rho\alpha) - I_{\nu}(\rho\alpha)K_{\nu+1}(\rho\alpha)]}
\]

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:

\[
\frac{i}{\alpha} \cdot \frac{J_{\nu+1}^2(\alpha) - J_{\nu+1}^2(\rho\alpha)}{J_{\nu+1}(\alpha) \cdot J_{\nu+1}(\rho\alpha)}
\]

and the numerator can be likewise transformed into
\[
\frac{\eta}{2} \{ Y_{\nu+1}(\rho \alpha) J_{\nu}(\alpha x) - Y_{\nu}(\alpha x) J_{\nu+1}(\rho \alpha) \}
\]

\[ F_{II}(x, \rho, \alpha) \text{ can thus be given as } \]
\[
F_{II}(x, \rho, \alpha) = \frac{\eta \pi}{2} J_{\nu+1}(\alpha) J_{\nu+1}(\rho \alpha) \frac{\{ J_{\nu}(\alpha x) Y_{\nu+1}(\rho \alpha) - Y_{\nu}(\alpha x) J_{\nu+1}(\rho \alpha) \}}{\{ J_{\nu+1}(\alpha) - J_{\nu+1}(\rho \alpha) \}}
\]

Thus the inverse of \( u_{II} \) is:
\[
U_{II} = L^{-1}\{ u_{II} \} = (Q-2\nu) \left[ \frac{2(\nu+1)x^{2\nu}}{\rho^{2\nu+1}-1} \theta \tau - \frac{\rho^2(\nu+1)x^{2\nu}-\rho^{2\nu}}{2\nu \rho^{2\nu+2}-1} \right] + \frac{x^{2\nu+2}}{2(\rho^{2\nu+2}-1)} \left[ \frac{1-\rho^{2\nu+4}}{2\nu+4} + \frac{\rho^2(\nu+1)}{2\nu} \right] + \frac{2(\nu+1)x^{2\nu}(B-1)(1-e^{-B\lambda \tau})}{(\rho^{2\nu+2}-1)\theta \beta^2 \lambda} + \sum_{n=1}^{\infty} 2F_{II}(x, \rho, \alpha) \left[ \frac{e^{s_{n_1}T}(s_{n_1}+\lambda)^2}{\Theta_{n_1}\{ (s_{n_1}+\lambda)^2 + (B-1)\lambda^2 \}} + \frac{e^{s_{n_2}T}(s_{n_2}+\lambda)^2}{\Theta_{n_2}\{ (s_{n_2}+\lambda)^2 + (B-1)\lambda^2 \}} \right]
\]

In analogy with the above derivation of \( U_{II} \) it can be shown that the inverse transform of \( u_{III} \) is given by:
\[
U_{III} = L^{-1}\{ u_{III} \} = 2\nu \left[ \frac{2(\nu+1)x^{2\nu}}{\rho^{2\nu+1}-1} \theta \tau - \frac{\nu(\nu+1)x^{2\nu}-1}{2\nu \rho^{2\nu+2}-1} \right] + \frac{x^{2\nu+2}}{2(\rho^{2\nu+2}-1)} \left[ \frac{1-\rho^{2\nu+4}}{2\nu+4} + \frac{\rho^2(\nu+1)}{2\nu} \right] + \frac{2(\nu+1)x^{2\nu}(B-1)(1-e^{-B\lambda \tau})}{(\rho^{2\nu+2}-1)\theta \beta^2 \lambda} + \sum_{n=1}^{\infty} 2F_{III}(x, \rho, \alpha) \left[ \frac{e^{s_{n_1}T}(s_{n_1}+\lambda)^2}{\Theta_{n_1}\{ (s_{n_1}+\lambda)^2 + (B-1)\lambda^2 \}} + \frac{e^{s_{n_2}T}(s_{n_2}+\lambda)^2}{\Theta_{n_2}\{ (s_{n_2}+\lambda)^2 + (B-1)\lambda^2 \}} \right]
\]

where \( F_{III}(x, \rho, \alpha) = \frac{\eta \pi}{2} J_{\nu+1}(\alpha) \{ J_{\nu}(\alpha x) Y_{\nu+1}(\rho \alpha) - Y_{\nu}(\alpha x) J_{\nu+1}(\rho \alpha) \} \)

\[ \frac{J_{\nu+1}(\alpha) Y_{\nu+1}(\rho \alpha) - Y_{\nu}(\alpha x) J_{\nu+1}(\rho \alpha)}{J_{\nu+1}(\alpha) - J_{\nu+1}(\rho \alpha)} \]
Combining $U_I$, $U_{II}$ and $U_{III}$ finally gives the solution for $U$ sought for:

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

$$Q \left[ \frac{2(\nu+1)x^{2\nu}}{\rho^{2\nu+2} - 1} \right] \sum_{n=1}^{\infty} \frac{x^{2\nu}(x^2 - \rho^2)}{2(\rho^{2\nu+2} - 1)} + \frac{\rho^2(\rho^{2\nu} - x^{2\nu})}{2\nu(\rho^{2\nu+2} - 1)} + \frac{\rho^2(\rho^{2\nu} - 1)x^{2\nu}(\nu+1)}{2\nu(\rho^{2\nu} - 1)^2} +$$

$$+ \frac{x^{2\nu}(\nu+1)(1-\rho^{2\nu+4})}{(2\nu+4)(\rho^{2\nu+2} - 1)^2} + \frac{2(\nu+1)x^{2\nu}(\nu - 1)(1 - e^{-3\lambda^2})}{(\rho^{2\nu+2} - 1)\Theta^2 \lambda} +$$

$$+ \sum_{n=1}^{\infty} \frac{s_{n1} \tau}{e^{n1(\frac{s_{n1} + \lambda}{2})^2}} + \frac{s_{n2} \tau}{e^{n2(\frac{s_{n2} + \lambda}{2})^2}} \}$$

(A-16)

with

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

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

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

and

$$s_{n1,2} = \frac{-(\lambda \Theta + \alpha^2)}{2\Theta} \pm \sqrt{(\lambda \Theta + \alpha^2)^2 - 4\lambda \alpha^2}$$

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

$$\lim_{\lambda \to \infty} s_{n2} = -B\lambda$$

and so:

$$\lim_{\lambda \to \infty} s_{n2} \Theta (\frac{s_{n2} + \lambda}{2}) = 0$$
As \( s_{n_1} \cdot s_{n_2} = \frac{\lambda \alpha^2}{\Theta} \) it follows that \( \lim_{\lambda \to \infty} s_{n_1} = -\frac{\alpha^2}{\Theta} \)

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

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

The solution for instantaneous adsorption is thus:

\[
U = \left( \frac{\rho^2 - 1}{\rho^{2v+2} - 1} \right) (\nu+1)x^{2v} \\
+ Q \left\{ \frac{2(v+1)x^{2v}}{\rho^{2v+2} - 1} + \frac{x^{2v}(\Delta^2 - \rho^2)}{2v(\rho^{2v+2} - 1)} + \frac{\rho^2(\Delta^2 - x^{2v})}{2v(\rho^{2v+2} - 1)} + \frac{\rho^2(\rho^{2v-1})x^{2v}(\nu+1)}{2v(\rho^{2v+2} - 1)} \right\} \\
+ \frac{x^{2v}(\nu+1)(1-\rho^{2v+1})}{(2v+4)(\rho^{2v+2} - 1)^2} \\
+ (Q-2v)x^{\nu} \pi \sum_{n=1}^{\infty} \exp \left( \frac{-\alpha^2 \tau}{\nu+1} \right) \frac{J_{\nu+1}(\alpha_n)^2 J_{\nu+1}(\alpha_n)}{\Theta} \frac{\alpha_n \{J_{\nu+1}(\alpha_n) - J_{\nu+1}(\alpha_n)\}}{\alpha_n \{J_{\nu+1}(\alpha_n) - J_{\nu+1}(\alpha_n)\}} \\
+ \frac{2v\nu x^{\nu}}{\rho^{\nu+1}} \sum_{n=1}^{\infty} \exp \left( \frac{-\alpha^2 \tau}{\nu+1} \right) \frac{J_{\nu+1}(\alpha_n)^2 J_{\nu+1}(\alpha_n)}{\Theta} \frac{\alpha_n \{J_{\nu+1}(\alpha_n) - J_{\nu+1}(\alpha_n)\}}{\alpha_n \{J_{\nu+1}(\alpha_n) - J_{\nu+1}(\alpha_n)\}} \\
+ \frac{2v\nu x^{\nu}}{\rho^{\nu+1}} \sum_{n=1}^{\infty} \exp \left( \frac{-\alpha^2 \tau}{\nu+1} \right) \frac{J_{\nu+1}(\alpha_n)^2 J_{\nu+1}(\alpha_n)}{\Theta} \frac{\alpha_n \{J_{\nu+1}(\alpha_n) - J_{\nu+1}(\alpha_n)\}}{\alpha_n \{J_{\nu+1}(\alpha_n) - J_{\nu+1}(\alpha_n)\}} (A-17)
\]

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 \( \nu \) is a factor in the denominator:

\[
\lim_{\nu \to 0} \frac{\rho^2(\rho^{2v} - x^{2v})}{2v(\nu+2v+2-1)} = \rho^2 \lim_{\nu \to 0} \frac{e^{2\nu \ln \rho - 2\nu \ln x}}{2v} = \rho^2 \lim_{\nu \to 0} \frac{1 + \nu \ln \rho + (2\nu \ln \rho)^2/2 + \ldots - 1 - 2\nu \ln x - \ldots \ldots} {2v} \\
\lim_{\nu \to 0} \frac{\rho^2}{\rho^{2v-1}} \frac{\ln \rho + o(\nu)}{x} = \frac{\rho^2}{\rho^{2v-1}} \frac{\ln \rho}{x}
\]

\[
\frac{\rho^2}{\rho^{2v-1}} \lim_{\nu \to 0} \frac{\ln \rho + o(\nu)}{x} = \frac{\rho^2}{\rho^{2-1}} \frac{\ln \rho}{x}
\]
and

\[
\lim_{\nu \to 0} \frac{\rho^2 (\rho^2 V - 1) x^2 (\nu + 1)}{2 \nu (\rho^2 + 2 - 1)^2} = \frac{\rho^2}{(\rho^2 - 1)^2} \lim_{\nu \to 0} \frac{2 \nu \ln \nu + (2 \nu \ln \nu)^2}{2!} + \ldots
\]

\[
= \frac{\rho^2}{(\rho^2 - 1)^2} \ln \nu
\]

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

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

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

\[
\xi = \frac{\alpha_n J_1 (\alpha \cdot \nabla) J_1 (\rho \alpha_n) \{ J_1 (\alpha \cdot \nabla) Y_1 (\rho \alpha_n) - Y_1 (\alpha \cdot \nabla) J_1 (\rho \alpha_n) \}}{2 \{ J_1^2 (\alpha \cdot \nabla) - J_1^2 (\rho \alpha_n) \}}
\]

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:

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

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 \( \nu \) from (A-2) and (A-9) and find \( V \) as \( L^{-1} \{ \nu \} \) in a similar way as \( U \) was found as \( L^{-1} \{ u \} \). It is easier however to write \( V \) as:

\[
V = L^{-1} \left\{ \frac{\lambda}{s + \lambda} u \right\} + \exp^{-\lambda \tau}
\]
and find \(L^{-1}\left\{\frac{\lambda}{s+\lambda}u\right\}\) with the convolution theorem:

\[
L^{-1}\left\{\frac{\lambda}{s+\lambda}\right\} = \int_0^T U(t,x)\lambda e^{-\lambda(t-x)} \, dz \tag{A-20}
\]

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 \(\tau\), and represented by \(f(x)\). The convolution integral for these terms is:

\[
\int_0^T f(x)\lambda e^{-\lambda(t-z)} \, dz = f(x)(1-e^{-\lambda T})
\]

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

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

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

\[
\int_0^T \lambda p(x)(1-q) e^{-\lambda(t-z)} \, dz = \int_0^T p(x)e^{-\lambda \tau} \left[ e^{\lambda z}\frac{-e^{-B(1-B)\lambda z}}{1-B} \right]_0^T = p(x)\left(1 - \frac{e^{-B\lambda T}}{1-B} + \frac{Be^{-\lambda \tau}}{1-B} \right)
\]

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:

\[
\int_0^T r(x,s) e^{-\lambda(t-z)} \, dz = r(x,s)\lambda \frac{(s e^{-\lambda T} - e^{-\lambda T})}{(s + \lambda)^2}
\]

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 Bessel functions

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

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

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

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

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

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

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

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

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

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. \( \frac{d}{dz} I_{\nu}^0(z) = z I_{\nu-1}(z) \)

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

p13. \( J_\nu(z)Y_\nu^\prime(z) - Y_\nu(z)J_\nu^\prime(z) = \frac{2}{\pi z} \)
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 Bessel functions 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 preliminary 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 $t(160)$ the values of $\alpha_n$, $s_1^n$, $s_2^n$, and the corresponding terms from the series in 15c and 15d. It can be seen that with increasing $\alpha_n$ the value of $s_2^n$ tends to $\alpha_n^2/\theta$, and that of $s_1^n$ to $\lambda(1.44406 \times 10^{-04})$ as follows from (A-13) and (A-14) in appendix I.
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C ******************** INPUT OF PARAMETERS ***********************

C 0011 TYPE 701
0012 701 FORMAT(Ix,'GIVE EVAP')
0013 ACCEPT 300,EVAP
0014 TYPE 301
0015 301 FORMAT(Ix,'GIVE EII EN NIW')
0016 ACCEPT 300,BIW,FIW
0017 BIW=BIW
0018 NIW=FIW
0019 TYPE 202
0020 202 FORMAT(Ix,'GIVE CI')
0021 ACCEPT 300,CI
0022 TYPE 203
0023 203 FORMAT(Ix,'GIVE IT,NT')
0024 ACCEPT 300,BIT,FIT
0025 IT=BIT
0026 NI=FIT
0027 2 TYPE 201
0028 201 FORMAT(Ix,'GIVE HALF')
0029 ACCEPT 300,HALF
0030 300 FORMAT(F,10.0)

C EVAP = EVAPORATION RATE CM/DAY , CI INITIAL CONCENTRATION MG/ML
C HALF = HALFTIME ADSORPTION RFACTION DAY
0031 DD 700,IN=W,JW,NIW
0032 RDENS=W(IW)

C ******************** CALCULATION DIMENSIONLESS GROUPS ****************

C 0033 ETA=HSC/R0
0034 R=AK/WC+1
0035 TNU=EVAP/(2.*PI*ETA*R0*RDENS*DACC)
0036 ORD=TNU/2
**FORTRAN IV**

```fortran
0037  ORD1=ORD1+1.
0038  R1=1./SQR(PI*RDENS).
0039  RHO=R1/R0.
0040  ALAB=ALOG(2.)/HALFT*R0*R0/DACC.
0041  PHI=DACC*C1/(AAA*R0).
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 ZEJNU(A,I,RHO,ORD,20.,I,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,1)=(-A2*SQRT(DISC))/(2.*WC).
0049  S(I,2)=S(I,1)**2/(A2+SQRT(DISC)).
0050  10 CONTINUE.

C
C  WRITE(1,400) (I,ALPH(I),S(1,1),S(1,2),I=1,N).
0051  400 FORMAT(IH0,'I',I1X,'ALPH',I1X,'S1',I1X,'S2'.
0052  $1X,'I',13X,'S1',I1X,'S2'.

C
C  WRITE(1,500) AK,WC,DACC,R0,NDENS,ALAB,RHO,TAU,PHI,Q.
0053  500 FORMAT(IH0,'PARAMETERS'.
0054  $1X,'AK','=1PE15.5',I1X,'ML/CM3'.
0055  $1X,'WC','=1PE15.5',I1X,'ML/CM3'.
0056  $1X,'DACC','=1PE15.5',I1X,'CM2/DAY'.
0057  $1X,'RO','=1PE15.5',I1X,'CM'.
0058  $1X,'RDENS','=1PE15.5',I1X,'CM-2'.
0059  $1X,'ALAB','=1PE15.5',I1X,'RHO','=1PE15.5'.
0060  $1X,'TAU','=1.',I1X,'Q'.

C
C  ***********************************  CALCULATION TAU'C  ***********************************

0061  DELX=(RHO-1.)/5.
0062  SUMR=STRA(1.0).
0063  P1=2.*ORD1/(RHO**(TN+2.))*-1.0.
0064  P1=P1/(B*WC).
0065  FST=(RHO/RHO-1.).
0066  G/(RHO**(TN+2.))*-1.0*ORD1*1.**TN.
0067  TAU'C=1./P1*(FST/G+SUMR).
0068  DO 80 J=1,6.
0069  X=1.+DELX*(J-1.).
0070  FST=(RHO*RHO-1.).
0071  G/(RHO**(TN+2.))*-1.0*ORD1*1.**TN.
0072  U(J)=STRA(X,TAU'C)*G+FST.
0073  80 CONTINUE.
0074  WRITE(1,800).
0075  800 FORMAT(IH0,'TAU',U(TAU'C) IN CASE OF steady-RATE').
0076  WRITE(1,800)TAU,1.)*U(J),J=1,6.
0077  QTAU=1.
```

---

This FORTRAN IV code snippet calculates various coefficients and parameters, including the calculation of zeros of crossproducts of Bessel functions and the calculation of Tau, among other things. The code is structured with DO loops and various mathematical operations to achieve these calculations. The final output includes formatted results for different parameters and coefficients, clearly indicating the code's purpose in numerical calculations, possibly for physics or engineering applications.
C *************** CALCULATION COMPLETE SOLUTION ***************

DO 70 ITIM=IT,NIT
DO 70 J=1,N

TAU=BACC*TIM(ITIM)/(RO*RO)
EXPL=EXP(-ALAB*TAU)

X=1.*DELX*(J-1)
IX=X

XTNU=X**TNU

DIST(J)=X

0TERM1=1.
SUM1=0.
SUM2=0.
VSUM1=0.
VSUM2=0.

C *************** CALCULATION OF SERIES ***************

DO 40 I=1,N

IF(DTAU,ER,TAU)GO TO 41

A=ALPH(I)
RA=RHO*A
AX=AXX

CALL BESFJ(A,ORD1,7,BJ)
JN1A=BJ(C2)
JNXA=BJ(1)

CALL BESFJ(RA,ORD1,7,BJ)
JN1RA=BJ(1)
YNXA=BY(1)

CALL BESFJ(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

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
EX2=EXP(E2)*FAC2

ARG2(I)=EX1+EX2

TERM1(I)=ARG1(I,J)*ARG2(I)
```fortran
FORTRAN IV V02.5 THU 25-JUN-81 12:40:15
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))*ALAR
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
0119 TERM1=TERM1(I)
0120 SUM1=SUM1+TERM1(I)
0121 SUM2=SUM2+TERM2(I)
0122 SUM1=VSUM1+VTERM1
0123 VSUM1=VSUM1+VTERM2
0124 IF(ABS(TERM1(I))/SUM1),LE,1,E-9) GO TO 50
0125 40 CONTINUE
0130 50 CONTINUE

C ******************* STEADY-STATE PART *******************

0131 FST=(RHO*RHO-1,)
    *(RHO**2*(TNU+2i)-1i)*ORD1**TNU

C ******************* STEADY-RATE PART *******************

0132 USTR=STRA(X,TAU)*F0
0133 USRA=Q0
0134 P(I)=P(1)+(ALAB*TAU)*(EXP(-ALAB*TAU)-1i)
0135 EXPD=1i-EXP(-B*ALAB*TAU)/(1i-B)+B*EXP(B)/(1i-B)
0136 P(6)=2*ORD1**TNU**(B-1i)*EXPD/
    (DENOM*W*C*B*ALAB)
0137 DO 89 I=2,5
0138 P(I)=P(I)*(1i,EXPL)
0139 89 CONTINUE
0140 DO 90 I=1,6
0141 USTRA=USTRA+P(I)
0142 90 CONTINUE
0143 VSTR=USTRA
0144 USUM1=USUM1**(D-TNU)**ORD
0145 USUM2=USUM2*TNU**ORD/(RHO**ORD1)
0146 USUM1=USUM1**(Q-TNU)**ORD
0147 SUM2=SUM2*TNU**ORD/(RHO**ORD1)

C ******************* TOTAL SOLUTION *******************

0148 U(J)=USTRA+SUM1+SUM2+FST
0149 U(J)=USTRA+USUM1+USUM2+FST*(1i,EXPL)+EXPL
0150 WRITE(1,402) X,SUM1,SUM2,USTRA,FST
0151 WRITE(1,402) X,USUM1,USUM2,VSTR,FST
0152 402 FORMAT(1HO,`X=`'PE15.5',2X,`SUM1='PE15.5,
    12X,’SUM2='PE15.5,2X,’USTRA='PE15.5,2X,’FST='PE15.5)
0153 30 CONTINUE
0154 OTAU=TAU
0155 WRITE(1,601) TAU(J),DIST(J),U(J),V(J),J=1,6
0156 600 FORMAT(1HO,`TAU='PE15.5/
    11X,`J=',1X,`DIST=',14X,’U'/1X,I2,'IP215.5))
0157 601 FORMAT(1HO,`TAU='PE15.5/
`````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````````
11X,'J',11X,'DIST',14X,'U',14X,'U'/((1X,I2,1P3E15.5))
0159     IF(U(1).LT.0..OR.TAU.GT.ABS(TAUC))GO TO 700
0160     CONTINUE
0161     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'.

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**FORTRAN IV STORAGE MAP FOR PROGRAM UNIT MAIN.**

**SUBROUTINES, FUNCTIONS, STATEMENT AND PROCESSOR-DEFINED FUNCTIONS:**

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FUNCTION STRA(X, TAU)

COMMON /PAR/ RHO, DENOM, B, WC, ALAB, ORD, TNU, ORD1, P

RH02 = RHO** (TNU + 2)
DENOM = 1. - RH02

RH02 = RHO** (TNU + 2)
DENOM = -DENOM
XNU = X**TNU
P(1) = 2. * ORD1 * XNU * TAU / (WC * B * DENOM)
P(2) = XNU * (X**RH02 - RH02) / (DENOM)
P(3) = RH02 * RH02 * (RH02 * TNU - 1) / (TNU * DENOM * DENOM)

$XNU*ORD1
P(5) = XNU * ORD1 * (1 - RH02 * (TNU + 4)) / (*DENOM * DENOM * (TNU + 4))

IF(ALAB .LE. 0.) GO TO 2
IF(ABS(B * ALAB * TAU) .GT. 87.) GO TO 3
EXPL = EXP(-B * ALAB * TAU)
GO TO 4
CONTINUE

P(6) = 2. * ORD1 * XNU * (B - 1.) * (1. - EXPL) / $(DENOM * WC * B * ALAB)
CONTINUE

WRITE(1, 500) P
500 FORMAT (1HO, 'TERMEN UIT STEADY-RATE !/'
(1P4E15.5))
STR = 0.
DO 1 I = 1, 8
STR = STR + F(I)
1 CONTINUE
RETURN
END
### LOCAL VARIABLES, PSECT $DATA, SIZE = 000060 (24 WORDS)

<table>
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<tr>
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<td>I</td>
<td>I*2</td>
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### COMMON BLOCK /PAR /, SIZE = 000070 (28 WORDS)

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<td>R*4</td>
<td>000000</td>
<td>DENOM</td>
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<td>R*4</td>
<td>000030</td>
<td>ORD1</td>
<td>R*4</td>
<td>000034</td>
<td>P</td>
<td>R*4</td>
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### LOCAL AND COMMON ARRAYS:

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<tr>
<td>P</td>
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<td>PAR 000040</td>
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### SUBROUTINES, FUNCTIONS, STATEMENT AND PROCESSOR-DEFINED FUNCTIONS:

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