A three-region analytical model of solute leaching in a soil with water-repellent top layer

Gerrit H. de Rooij
ABSTRACT

When water infiltrates into a soil with a water-repellent top layer, the wetting front breaks up into fingers, enhancing solute leaching to the groundwater. In a recent paper, the flow pattern associated with fingering was divided into three regions. In the top few centimeters, water radially flows towards the finger tops. Then, it will move vertically downwards through the actual fingers towards the bottom of the water-repellent layer. In the wettable subsoil, matric forces will cause the flow lines to diverge. This report presents analytical solutions for each of the three regions. They allow the calculation of the break-through of a pulse of an inertious solute not subject to diffusion or dispersion. Tentative calculations show the flow pattern yields a tailed break-through curve (BTC). The wettable layer dominates the shape of the BTC. A thin distribution zone gives a steep cumulative BTC. Increasing the radial dimensions of the system yields pronounced tailing of the BTC. The model offers a new, possibly fruitful, approach to model fingering. To correctly predict solute leaching, calibration of the properties of the distribution zone and the finger appears to be required.
INTRODUCTION

Water will only enter a water-repellent soil when the pressure head is non-negative. Hence, the location on which infiltration occurs will be saturated and the soil hydraulic conductivity equal to that at saturation. Especially in sandy soils, the saturated conductivity will usually exceed the precipitation rate and the flow will only occupy part of the soil matrix [e.g. Raats, 1973; Hillel and Baker, 1988]. This process is usually termed fingering and the preferential flow paths fingers. Since the soil surrounding these fingers hardly participates in the flow, fingering enhances the leaching of solutes to the groundwater. It also limits the opportunities for adsorption and degradation of organic compounds [Hillel, 1987; Glass et al., 1988; Steenhuis et al., 1990; Gee et al., 1991].

The flow pattern associated with fingering is complex. Three regions with markedly different flow characteristics can be distinguished. In the top few centimeters of a soil with a water-repellent top layer, water flows laterally towards the fingers. Hence, the flow converges in this layer. Within the fingers, the water moves vertically until it reaches the wettable subsoil. There, the flow diverges again due to capillary forces. Ritsema et al. [1993] first presented this concept.

This report presents an analytical, steady-state model of this flow system. The model offers several new possibilities:
- it permits the calculation of the BTC of an inertious solute not subject to diffusion or dispersion,
- the way each of the flow regions affects the BTC can be quantitatively evaluated,
- it allows identification of the soil and flow characteristics that most strongly affect solute leaching.

The latter point is of interest in the development of more detailed numerical models.

The properties of a soil in the Dutch coastal dune area near Ouddorp (Sandy Mesic Typic Psammaquent) were used in the calculations that illustrate these points. The soil was selected for the strong water-repellency of its top layer and its high saturated conductivity [van Ommen et al., 1989; van Dam et al., 1990; Hendrickx and Dekker, 1991, with personal communication of L.W. Dekker, 1991; Ritsema et al., 1993].
The model describes the flow associated with one finger. Radial symmetry is assumed. Figure 1 outlines the model and defines the three regions. Either no mixing or full mixing can occur in the distribution zone and the finger. No mixing is assumed in the wettable soil. This results in the following cases considered:

Case I: No mixing in any region.
Case II: Full mixing in the distribution zone, no mixing in the other regions.
Case III: Full mixing in the finger, no mixing in the other regions.
Case IV: Full mixing in the distribution zone and the finger, no mixing in the wettable soil.

Figure 1. The flow pattern associated with one finger. The dashed lines denote the boundaries between the three flow regions. The central stream line is the axis of radial symmetry.
2.1 The distribution zone

This term is adopted from Ritsema et al. [1993] to identify the region just below the soil surface in which water flows towards the fingers. The water content and thickness of this layer are assumed uniform. The radial velocity of the water is determined by the infiltration upstream of and the area of flow at the radius under consideration:

\[
v_r(r) = -\frac{P\pi(R^2-r^2)}{2\pi r L_d \theta_d} = -\frac{P}{2L_d \theta_d} \cdot \frac{R^2-r^2}{r}
\]

where \(v_r\) is the radial flow velocity (m d\(^{-1}\)), \(r\) is the radius (m), \(R\) is the radius of the circular micro-catchment of the finger (m), \(P\) is the precipitation rate (m d\(^{-1}\)), \(L_d\) is the thickness of the distribution zone (m), and \(\theta_d\) is its volumetric water content (-). For uniform flow within the finger, the radius at which a parcel of water enters the finger is:

\[
r_f = \frac{R_f}{R} \cdot r_i
\]

where \(r_f\) is the radius of a stream tube within the finger (m), \(r_i\) is the radius at which the parcel of water infiltrated (m), and \(R_f\) is the finger radius (m). The shape of the finger top that protrudes into the distribution zone is such that a streamline is intercepted without affecting the ones above it. At a given radius, the height above the bottom of the distribution zone of an infiltrated parcel of water is determined by the amount of infiltration 'upstream' of \(r_i\) (flowing underneath the parcel) and between \(r_i\) and the current radius (flowing above the parcel). With equation (2), the height of the finger top as a function of \(r\) becomes:

\[
E_f = \frac{R^2-R_f^2}{R_f^2} \cdot \frac{R^2-r^2}{R^2-r_i^2} \cdot L_d
\]

where \(r\) ranges from 0 to \(R_f\). \(E_f\) denotes the height of the protrusion of the finger top (m). With \(v_r = \frac{dr}{dt}\) and separation of variables, equation (1) can be integrated between \(r_i\) and \(r_f\) to yield:

\[
t_d(x_i) = \frac{L_d \theta_d}{P} \ln \left( \frac{R^2-x_i^2}{R^2-r_i^2} \right)
\]

where \(t_d\) is the travel time in the distribution zone (m). Inverting this
relationship gives the radius of infiltration associated with a given travel time:

\[ r_j = R \left[ \exp \left( \frac{P_t d}{L_d i_d} \right) - 1 \right] \frac{1}{2} \left( \exp \left( \frac{P_t d}{L_d i_d} \right) - \frac{R_f^2}{R^2} \right) \]  

(5)

For a solute pulse \( I \) (kg), applied uniformly to the soil surface, the amount of solute delivered to the finger by the region within \( r_f \) is:

\[ S(r) = \frac{I}{R^2} \cdot r_f^2 \]  

(6)

with \( S \) the total amount of solute stemming from the region bounded by \( r \) (kg). For cases I and III (no mixing in the distribution zone), the BTC at the interface between the distribution zone and the finger is:

\[ \frac{\partial S}{\partial t} = \frac{\partial S}{\partial r_f} \frac{dr_f}{dt} \]  

(7)

Taking the derivative of equation (5) yields:

\[ \frac{dr_f}{dt_d} = \frac{1}{2} \frac{PR}{L_d \theta_d} \left( 1 - \frac{R_f^2}{R^2} \right) \exp \left( \frac{P_t d}{L_d i_d} \right) \left[ \exp \left( \frac{P_t d}{L_d i_d} \right) - 1 \right] \frac{1}{2} \left[ \exp \left( \frac{P_t d}{L_d i_d} \right) - \frac{R_f^2}{R^2} \right]^{\frac{3}{2}} \]  

(8)

Inserting (8) and the derivative of (6) in (7), and subsequently expressing \( r_f \) in terms of \( t_d \) using (5) gives:

\[ q^S(t) = \frac{IP}{L_d \theta_d} \left( 1 - \frac{R_f^2}{R^2} \right) \exp \left( \frac{P_t d}{L_d \theta_d} \right) \left[ \exp \left( \frac{P_t d}{L_d \theta_d} \right) - \frac{R_f^2}{R^2} \right]^{\frac{3}{2}} \]  

(9)

where \( q^S \) is the solute flux across the interface between the distribution zone and the finger (kg d\(^{-1}\)). The cumulative break-through is obtained by integration:
\[ S(t) = \int_0^t q^* dt \]
\[ = \frac{I}{\exp\left(\frac{P t}{L_d \theta_d}\right) - 1} \exp\left(\frac{P t}{L_d \theta_d}\right) - \frac{R^2_t}{R^2} \exp\left(\frac{P t}{L_d \theta_d}\right) - \frac{R^2_t}{R^2} \] \hspace{1cm} (10)

Since the distribution zone is thin, mixing is likely. If the solute pulse is immediately distributed over the entire volume of the distribution zone, each stream tube starts to deliver solute to the finger at the time of application \((t = 0)\), and continues to do so until its travel time is exceeded. With the volume of the distribution zone calculated using equation (3), the solute concentration at \(t = 0\) is:

\[ c_d = \frac{I}{\pi L_d \theta_d R^2} \cdot \frac{R^2}{R^2 - R^2_t} \left[ \ln\left(\frac{R^2}{R^2 - R^2_t}\right) \right]^{-1} \] \hspace{1cm} (11)

where \(c_d\) is the solute concentration in the distribution zone \((\text{kg m}^{-3})\). At any given time \(t\), solute is delivered to the finger from the area between \(R\) and the radius of infiltration having a travel time equal to \(t\). The water flux carrying solute follows from \(r\) and \(P\). With \(r\) obtained from equation (5), the BTC at the interface between the distribution zone and the finger becomes, for cases II and IV (full mixing in the distribution zone):

\[ q^*(t) = c_d P \pi [R^2 - r(t)^2] \]
\[ = \frac{IP}{L_d \theta_d} \cdot \frac{R^2_t}{R^2 - R^2_t} \cdot \left[ \ln\left(\frac{R^2_t}{R^2 - R^2_t}\right) \right]^{-1} \left[ 1 - \frac{\exp\left(\frac{P t}{L_d \theta_d}\right) - 1}{\exp\left(\frac{P t}{L_d \theta_d}\right) - \frac{R^2_t}{R^2}} \right] \] \hspace{1cm} (12)

Integration yields the cumulative break-through:
\[ S(t) = \int_{0}^{t} q^* \, dt \]

\[ = \frac{IP}{L_d \theta_d} \cdot \frac{R_t^2}{R^2 - R_t^2} \left( \ln \frac{R_t^2}{R_t^2 - R_f^2} \right)^{-1} \left\{ \left( 1 - \frac{R_t^2}{R_f^2} \right) t + \frac{L_d \theta_d}{P} \left( \frac{R_t^2}{R_f^2} - 1 \right) \right\}. \]  

(13)

\[ \ln \left[ \frac{\exp \left( \frac{P \theta_d}{L_d \theta_d} \cdot \frac{R_t^2}{R^2} \right)}{1 - \frac{R_t^2}{R^2}} \right] \]

2.2 The finger

Flow through the finger is assumed uniform under unit gradient [e.g. Glass et al., 1989]. The water flux through the finger must be equal to the precipitation flux on the finger's micro-catchment. Hence, \( R_t \) and the soil hydraulic conductivity of the finger, \( K_f \) (m d\(^{-1}\)) have to be chosen such as to satisfy:

\[ R_t^2 \cdot K_f = R^2 \cdot P \]  

(14)

The travel time from finger top to bottom is directly proportional to the distance between the two. With equation (3):

\[ t_f(x_f) = \frac{\theta_f}{K_f} \left( L_f + \frac{R^2 - R_t^2}{R_t^2} x_f \right) \]  

(15)

with \( t_f \) the travel time (d) and \( \theta_f \) the water content (-) in the finger, and \( L_f \) the finger length (m). If no mixing in the finger is assumed, \( t_f \) at \( r_f \) has to be added to \( t_d \) at the corresponding \( r_t \). Combining (4) and (15) and taking \( r_t \) as the independent variable gives:

\[ t_{\theta f}(x_f) = \frac{L_d \theta_d}{P} \ln \left( \frac{R^2 - R_t^2}{R^2 - R_f^2} x_f \right) + \frac{\theta_f}{K_f} \left( L_f + \frac{R^2 - r_f^2}{R_t^2} \right) \]  

(16)

Because \( t_d \) is an increasing and \( t_f \) a decreasing function of \( r_t \), equation (16) cannot be inverted to yield \( dr_t/dt_f \). Since \( L_d \) is small compared to \( L_f \), replacing the term providing the height of the finger protrusion in the distribution zone by an equivalent uniform height has only a minor effect on
This equivalent height can be found by dividing the volume of the finger top (which can be calculated from equation [3]) by the area of the horizontal cross-section of the finger:

\[ E' = \frac{L_0 \pi R^2}{R^2} \left[ \left( 1 - \frac{R^2}{R^2} \right) \ln \left( \frac{R^2}{R^2-R^2} \right) + 1 \right] \]  

where \( E' \) denotes the equivalent uniform height of the protrusion of the finger top (m). The approximative total travel time becomes:

\[ t_{d,r'}(r_f) = \frac{L_0 \theta_f}{K_f} \ln \left( \frac{R^2-R^2}{R^2-r_f^2} \right) + \frac{\theta_f}{K_f} \left[ L_0 \frac{R^2}{R^2} \left( 1 - \frac{R^2}{R^2} \right) \ln \left( \frac{R^2}{R^2-R^2} \right) + 1 \right] \]  

with the prime indicating the approximative nature of the travel time. The last term on the right-hand side (RHS) gives the travel time in the finger. A new time coordinate is defined as:

\[ \tau' = \tau - \frac{\theta_f}{K_f} \left[ L_0 \frac{R^2}{R^2} \left( 1 - \frac{R^2}{R^2} \right) \ln \left( \frac{R^2}{R^2-R^2} \right) + 1 \right] \]  

The \( \tau' \) denotes the translated coordinate. Equation (18) differs from equation (4) by the right-hand term on the RHS only. Hence, \( dt/d\tau \) can be calculated by equation (8), with \( \tau' \) replacing \( \tau \). Therefore, the expressions for the BTC (equation [9]) and the cumulative break-through (equation [10]) remain valid for case I (no mixing anywhere) if \( \tau' \) is used. The same holds for equations (12) and (13), that give the BTC and the cumulative break-through for case II (full mixing in the distribution zone only). Clearly, if no mixing occurs in the finger and \( t_f \) is assumed independent of \( r_f \), the finger only delays solute break-through, without affecting the shape of the BTC.

In case of full mixing within the finger, the solute is redistributed horizontally, and the BTC at the finger bottom becomes independent of \( r_f \). If equation (18) is employed again, the BTC at the finger bottom has the same shape as that of the distribution zone, since the mixing regime in the finger does not affect travel times. Hence, if mixing does not occur in the distribution zone (case III), equations (9) and (10) are valid, and if it does (case IV), equations (12) and (13) hold. Here too, \( \tau' \) replaces \( \tau \).

The BTC and the cumulative break-through characterize solute transport in time. Also of interest is the break-through at the finger bottom as a function of \( r_f \). In the following, expressions are derived giving the total amount of solute \( S \) arriving in the area of the finger bottom bounded by a given radius. If possible, expressions linking the solute flux \( q^2 \) through the finger bottom to \( r_f \) will also be provided. In the case of mixing in neither the distribution zone nor the finger (case I), the solute pulse applied at the
soil surface results in a pulse output of each stream tube at the finger bottom. The arrival time of the pulse depends on \( r_f \) and is given by equation (18) if \( r_i \) is expressed in terms of \( r_f \). The spatial distribution of the solute pulse over the catchment area is reproduced at the finger cross-section. A uniform application will therefore give the following distribution of cumulative break-through within the finger (at \( t = \infty \)):

\[
\frac{\partial S}{\partial r_f} = \frac{2\pi}{R_f^2} r_f
\]  

(20)

The amount of solute delivered to the wettable zone by the area within \( r_f \) results from integration of equation (20):

\[
S(r_f) = \int_0^{r_1} \frac{\partial S}{\partial r_f} \, dr_f = \frac{I}{R_f^2} \cdot r_f^2
\]  

(21)

The solute delivered by an individual stream tube arrives as a pulse (infinitely large flux during an infinitesimal time interval), and the evaluation of the solute flux as a function of the radius is therefore meaningless.

If full mixing occurs in the distribution zone only (case II), a stream tube at radius \( r_f \) starts to deliver solute at the finger bottom at \( t^* = 0 \), and continues to do so for a time period \( t_d \) associated with the value of \( r_f \) corresponding to \( r_f \). To arrive at an expression for \( \partial q^w / \partial r_f \), it is necessary to consider the behavior of the water flux \( q^w (m^3 \text{d}^{-1}) \). In the distribution zone, \( q^w \) between \( r = 0 \) and \( r = r_f \) is:

\[
q^w(r_f) = P \cdot \pi r_f^2
\]  

(22)

The solute concentration is given by equation (11). Therefore:

\[
\frac{\partial q^s}{\partial r_f} = \frac{\partial q^w}{\partial r_f} \cdot c_d
\]

\[
= \frac{2\pi I x_f}{R^2 L \theta_d} \cdot \frac{R_f^2}{R^2 - R_f^2} \cdot \left[ \ln \left( \frac{R^2}{R^2 - R_f^2} \right) \right]^{-1}
\]  

(23)
With
\[ \frac{\partial q_s}{\partial x_t} = \frac{R}{R_t} \cdot \frac{\partial q_s}{\partial x_t} \] (24)

results:
\[ \frac{\partial q_s}{\partial x_t} = \frac{2P \xi_t}{L_d \theta_d (R^2 - R_t^2)} \left[ \ln \left( \frac{R^2}{R^2 - R_t^2} \right) \right]^{-1} \] (25)

Note the expression is time-independent. It gives the relationship between \( q_s \) and \( r_f \) while solute is delivered by the stream tube with radius \( r_f \). To arrive at the total amount of solute delivered by the stream tube, the flux has to be multiplied by the time period during which it occurs, i.e. \( t_d \) at the corresponding \( r_f \). This yields, for case II:
\[ \frac{\partial s_s}{\partial x_t} = \frac{2 \xi_t}{R^2 - R_t^2} \cdot \ln \left( \frac{R^2 - r_f^2}{R^2 - R_t^2} \right) \cdot \left[ \ln \left( \frac{R^2}{R^2 - R_t^2} \right) \right]^{-1} \] (26)

Integrating equation (26) between zero and \( r_f \) gives the amount of solute entering the wettable zone from the region bounded by \( r_f \):
\[ S(x_t) = \frac{I}{(R^2 - R_t^2) \ln \left( \frac{R^2}{R^2 - R_t^2} \right)} \]
\[ \cdot \left\{ \frac{r_f^2}{R^2} \ln \left( \frac{R_t^2}{R^2} \right) + R_t^2 \ln \left( \frac{R^2 - r_f^2}{R^2} \right) - R^2 \ln \left( \frac{R^2 - r_f^2}{R^2} \right) \right\} \] (27)

If full mixing occurs in the finger (cases III and IV), the BTC at the finger bottom becomes uniform over the finger area and \( \partial S/\partial x_t \) does not depend on the solute movement in the distribution zone any more. Since the entire solute pulse passes through the finger bottom uniformly, the behavior of \( S \) in time and space can be combined:
\[ \frac{\partial S}{\partial x_t} (x_t, t^*) = \frac{2S(R_t, t^*)}{R_t^2} \cdot x_t \] (28)
where $S(R_f, t^*)$ is given by equation (10) if mixing does not occur in the distribution zone (case III), and by equation (13) if it does (case IV). At a given shifted time $t^*$, the solute flux is given by equation (9) (case III) or (12) (case IV). Replacing $S(R_f, t^*)$ by $S(R_f, \infty) = I$ in equations (28) and (29) gives the distribution of the total solute break-through over the finger bottom. Like $S$, $q_s$ is also uniform over the finger cross-section, and the equations relating it to $r_f$ are analogous to equations (28) and (29) for $S$. $q(R_f, t^*)$ is given by either equation (9) (case III) or (12) (case IV).

2.3 The wettable soil

An exponential $K(h)$ relationship [Gardner, 1958] is assumed in the wettable soil:

$$K_w(h) = K_{w,s} \cdot e^{\alpha h}$$  

where $K_w$ is the hydraulic conductivity of the wettable soil (m d$^{-1}$), $\alpha$ is a soil-specific parameter (m$^{-1}$), and the subscript $s$ denotes the value at saturation. This allows the classical linearized form of Richards' equation to be used [Philip, 1969; Pullan, 1990]. With uniform flow through the finger, the finger bottom can be regarded a disc source above a shallow ground water table in a cylindrical flow domain, and the solution of de Rooij, Warrick, and Gielen [1994, in publication] applies. For our case, the solution reads:

$$\Phi(r, z) = \frac{K_{w,s} \cdot \exp[\alpha(z^*-L_w)]}{\alpha n R^2} + \frac{Q(1-\exp[\alpha(z^*-L_w)])}{\alpha n R^2}$$

$$+ \frac{8Q \exp[\frac{\alpha}{2} z^*]}{\pi a^2 R^4 R_f} \cdot \sum_{n=1}^\infty \frac{a \lambda_n R_f}{J_1(\frac{a \lambda_n R_f}{2})} \left(\frac{a \lambda_n R_f}{2 R_f}\right)$$

$$\cdot \exp\left(-\frac{a \mu_n z^*}{\mu_n + 1 + (\mu_n - 1) \exp(-a \mu_n L_w)}\right)$$

where $\Phi$ is defined as:
\[
\phi = \int_a^b \psi dh
\]  

(32)

In these equations, \(\phi\) denotes the matric flux potential \((m^2 d^{-1})\), \(h\) is the pressure head \((m)\), \(Q\) is the source strength \((m^3 d^{-1})\), \(z^* = z - L_d - L_f\) is the adjusted depth coordinate \((m)\), and \(L_w\) is the distance between the finger bottom and the groundwater table \((m)\), \(J_i(x)\) is the Bessel function of the first kind and order \(i\) of \(x\), and \(\lambda_n\) is calculated from the \(n^{th}\) non-zero positive root of:

\[
J_i\left(\frac{\alpha \lambda_n R}{2}\right) = 0
\]

(33)

\(\mu_n\) is defined by:

\[
\mu_n = \left(1 + \lambda_n^2\right)^{\frac{1}{2}}
\]

(34)

The source strength is:

\[
Q = \pi R^2 P
\]

(35)

The stream function was found using the method of Philip [1968] with some slight modifications to account for the non-zero source radius. The value of the stream function at a given point gives the flux contained by the stream tube passing through that point. It can be expressed in terms of either the vertical or the radial flux density. The expression in terms of the vertical flow requires the numerical evaluation of a definite integral of a Bessel function in each of the terms of an infinite sum. It was therefore discarded. The expression in terms of the radial flux density reads:

\[
f = \begin{cases} 
\frac{r^4}{R_f^4} - \frac{2\pi x}{Q} \int_0^{r'} v_z \theta \, dz^* & \text{for } r < R_f \\
1 - \frac{2\pi x}{Q} \int_0^{r'} v_z \theta \, dz^* & \text{for } r \geq R_f
\end{cases}
\]

(36)

where
Note that the expression was modified to let $f$ (-) denote the fraction of the total flow contained by a stream tube. To find the travel time along a stream tube defined by its value of $f$, the reciprocal of the flow velocity tangent to the tube has to be integrated along the tube. At a given point, the flow velocity can be found from the flux densities in the principal directions and the volumetric water content. The latter results from the pressure head (related to the matric flux potential) and the soil water retention curve. In this study, van Genuchten's [1980] expression for the retention curve is adopted:

$$\theta = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + (a|h|)^n\right]^{-\frac{1}{n}}}$$

(38)

where $a$ (L$^{-1}$) and $n$ (-) are shape parameters and the subscripts $r$ and $s$ denote the residual and saturated value of $\theta$, respectively. The flux density components are related to the matric flux potential as [Philip, 1968]:

$$v_x \theta = a \phi - \frac{\partial \phi}{\partial z}$$

(39)

$$v_z \theta = -\frac{\partial \phi}{\partial z}$$

(40)

where $v_x$ denotes the vertical flow velocity (m d$^{-1}$). Since this integration can only be carried out numerically, an expression relating the travel time in the wettable soil to $r_t$ cannot be given.
3 MATERIALS AND METHODS

3.1 The soil

In the calculations, the properties of a homogeneous sandy soil in the coastal dune area near Ouddorp in the south-western part of The Netherlands were employed. The soil is a mesic Typic Psammaquent with a water-repellent top-layer of ±0.2 m. The soil material is well sorted, with 1.9% of the mineral parts in the clay fraction (measured by the pipet-method) and 85.3% between 105 and 210 µm (measured by sieving) at 0.4-0.5 m below the soil surface (See Gee and Bauder [1986] for details on both methods). The organic matter content varies from 5.2% of the dry mass (0.1-0.2 m depth) to 0.3% (0.9-1.0 m depth) (weight loss after heating oven dry samples of 10 g to 950 degrees Celsius for 2.5 hrs).

The unsaturated conductivity was measured for pressure heads between -10 and -70 cm using the atomizer apparatus of Dirksen and Matula (1994) on an undisturbed soil column (0.2 m diam.) taken at 0.5-0.7 m depth (Agema, 1993). $K_w$ was obtained by extrapolation. $\theta_r$ was fixed on the measured value at a pressure head of $-10^6$ cm. $\theta_i$ was assumed equal to the porosity. The remaining parameters of the retention curve of the wettable soil were determined by inverse modeling of a multistep-outflow experiment on an 8 cm diam. soil core taken at 0.51-0.63 m depth (van Dam et al., 1992, 1994).

Table 1 summarizes the soil parameters.

<table>
<thead>
<tr>
<th>Variable and dimensions</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta_r$ (-)</td>
<td>0.0042</td>
</tr>
<tr>
<td>$\theta_i$ (-)</td>
<td>0.415</td>
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<tr>
<td>(Also valid for the</td>
<td></td>
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<tr>
<td>distribution zone and</td>
<td></td>
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<tr>
<td>the finger)</td>
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</tr>
<tr>
<td>$\alpha$ (m⁻¹)</td>
<td>2.26</td>
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<tr>
<td>$\beta$ (       )</td>
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<tr>
<td>$K_{w,s}$ (m d⁻¹)</td>
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<td>(Also valid for the</td>
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<td>distribution zone and</td>
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<td>the finger)</td>
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<tr>
<td>$\lambda$ (m⁻¹)</td>
<td>8.2</td>
</tr>
</tbody>
</table>

3.2 Sensitivity analysis

To identify the key parameters governing solute break-through given the soil described above, a sensitivity analysis was performed in which various system parameters were changed. Table 2 lists the parameters and their values. The combination of the median values yields field-representative reference conditions. The extreme values of each variable are within physically acceptable limits, except for $L_d$. Since this parameter is hard to measure, a large range was used to clearly show the effect. The selected
precipitation rates correspond to ten times the average net infiltration and to showers with a recurrence time of 0.2 yr and a duration of 60 and 15 minutes under Dutch conditions, respectively (Buishand and Velds, 1980). \( R_f \) was determined from \( P, R \), and the finger conductivity for each case. \( L_f \) was kept at 0.2 m in all simulations since the delay of the solute break-through caused by it can be easily calculated.

| Table 2. Values of system parameters used in the sensitivity analysis. |
|----------------|----------------|----------------|
| \( P \) (m d\(^{-1}\)) | \( R \) (m) | \( L_d \) (m) | \( L_w \) (m) |
| 0.010 | 0.11 | 0.01 | 0.50 |
| 0.173 | 0.25 | 0.05 | 0.75 |
| 0.389 | 0.40 | 0.10 | 1.20 |

4 RESULTS AND DISCUSSION

First, the effect of mixing on solute break-through was evaluated. Figure 2 shows the cumulative BTC for reference conditions for all mixing regimes. Since dispersion or diffusion were not included in the model, the curves may be interpreted as cumulative distribution curves of the travel time through the flow system. Since mixing in both the distribution zone and the finger is likely, the rest of the analysis will focus on case IV.

Figure 2. The effect of the mixing regime on solute leaching to the groundwater.

Next, the contribution of each of the regions to the cumulative BTC was determined. Figure 3 shows the cumulative BTC at the finger top (where the solute leaves the distribution zone), the finger bottom (where the solute leaves the finger), and at the groundwater level (where the solute leaves the wettable soil). Clearly, the shape of the cumulative BTC at the groundwater is largely determined by the wettable soil. Solute break-through only
slightly accelerated by fingering, as compared to stable, one-dimensional flow. On the other hand, the regions of low flow cause considerable tailing. These regions are located close to the bottom of the distribution zone and in the top of the wettable soil, in both cases near the flow domain radius.

Figure 3. The effect of each of the flow regions on solute breakthrough. The 1D-solution is for vertical infiltration in a similar soil without water-repellency in the top-layer.

While the BTC gives the distribution of solute over time, it is also interesting to see how fingering affects the solute distribution in space. Therefore, the total amount of solute leached within a given radius \( r \) was calculated for \( r \) between zero and \( R_j \). For one-dimensional flow, the fraction of the applied solute leaching within \( r \) would be directly proportional \( r^2 \). The result for reference conditions is given in Figure 4, together with the curve for 1D-flow. The effect of fingering appears to be negligible.
Increasing the precipitation rate retards the cumulative BTC due to increased storage in the wetter profile (Figure 5). It also steepens the curve since the flow better approximates 1D-flow under wet conditions because $R_f$ is larger and the regions of low flow become smaller. As a result, tailing reduces considerably with increasing precipitation rate. Increasing the domain radius (and the finger radius accordingly) flattens the cumulative BTC (Figure 6). Not surprisingly, the regions of low flow become more important for large radial dimensions.

Figure 4. The radial distribution of leached solute. Since the solute distribution at the finger bottom is non-uniform for case I only, it is presented separately.
Figure 5. Solute break-through as a function of cumulative drainage for different precipitation rates.

Figure 6. Cumulative solute break-through for different radial dimensions, as characterized by the flow domain radius.
A thin distribution zone gives a steep cumulative BTC with a prolonged tail. The curve becomes considerably smoother for large values of $L_d$ (Figure 7). For large wettable zones, the solute arrives later, but the cumulative BTC also becomes steeper since the flow better approximates 1D-flow (Figure 8). The time at which half of the applied solute has reached the groundwater appears to be a linear function of $L_w$ with intercept 0.196 and slope 1.60 d m$^{-1}$ ($R^2 = 1.00$). This indicates the water content in the top of the wettable soil is almost constant, resulting in a storage change that is proportional to the change in $L_w$.

![Figure 7. Cumulative solute break-through for various values for the thickness of the distribution zone.](image-url)
Figure 8. The effect of the thickness of the wettable soil (equal to the groundwater depth minus 25 cm) on solute leaching.
CONCLUSIONS

The model presented here has not yet verified on laboratory or field data. Nevertheless it offers a quantitative description of the full flow system associated with fingering in water-repellent soils. As such, it provides a new, potentially fruitful approach to model preferential flow.

Up to now, most efforts were directed towards modeling the actual finger. Measurements often focused on the formation and behavior of fingers. This model shows that the wettable soil below the finger is of much more importance for solute break-through under natural conditions. Together with the distribution zone, it yields a tailed break-through curve. In reality, diffusion of solute into the dry soil surrounding the fingers will enhance this effect.

The initial calculations presented here illustrate the major effect of the wettable zone on solute break-through. A thin distribution zone steepens the cumulative BTC. Increasing the radial dimensions of the system results in prolonged tailing, due to the increase of regions of very low flow in the wettable zone.

During the calculations, the distribution zone and the finger were assumed to be saturated. Assuming a saturated bottom layer in the distribution zone and modeling that according to Dupuit's assumptions does not allow an analytical expression for the BTC to be derived. Also, the distribution of the radial velocity did not deviate dramatically from that resulting from the simpler approach. The data of Ritsema et al. [1993] indicate that the water content in the distribution zone is considerably below saturation. The fingers appear to be even drier. Reducing the water content in the upper regions will reduce the hydraulic conductivity, and the reduced storage will be counteracted by an increase of the finger radius. Since the effect of both regions on the BTC is small, such a refinement of the model may not be worthwhile.

The behavior of the wettable soil largely determines solute break-through in a soil exhibiting fingering in a water-repellent top-layer. To adequately predict solute leaching in soils with water-repellent top-layers, a proper description of the flow in the wettable sub-soil may be more important than a detailed model of the actual fingers.
NOTATION

\( a \)  
shape parameter in equation (38), m\(^{-1}\)

\( c_d \)  
solute concentration in the distribution zone, kg m\(^{-3}\)

\( E_f \)  
height of finger top above the bottom of the distribution zone, m

\( E_f' \)  
equivalent height of finger top above the bottom of the distribution zone, m

\( f \)  
stream function, the fraction of the total flow contained by the given stream tube

\( h \)  
pressure head, m

\( H \)  
hydraulic head, m

\( I \)  
solute pulse applied at the soil surface, kg

\( J_i(x) \)  
Bessel function of the first kind and order \( i \) of argument \( x \)

\( K_d \)  
soil hydraulic conductivity of the distribution zone, m d\(^{-1}\)

\( K_f \)  
soil hydraulic conductivity within the finger, m d\(^{-1}\)

\( K_w \)  
soil hydraulic conductivity of the wettable soil, m d\(^{-1}\)

\( K_{w,s} \)  
soil hydraulic conductivity of the wettable soil at saturation, m d\(^{-1}\)

\( L_d \)  
height of the distribution zone, m

\( L_f \)  
finger height at \( R_f \), m

\( L_s \)  
thickness of the saturated zone in the distribution zone, m

\( L_w \)  
vertical distance between the finger bottom and the groundwater table, m

\( n \)  
shape parameter in equation (38)

\( P \)  
infiltration rate, m d\(^{-1}\)

\( Q \)  
source strength, m\(^3\) d\(^{-1}\)

\( q_s \)  
solute flux, kg d\(^{-1}\)

\( q_w \)  
water flux, m\(^3\) d\(^{-1}\)

\( r \)  
radius, m

\( r_f \)  
radius of a stream tube within the finger, m

\( r_i \)  
radius of infiltration, m

\( R \)  
radius of the flow domain, m

\( R_f \)  
finger radius, m

\( S \)  
total amount of solute arrived at a given region boundary, kg

\( t \)  
time, d

\( t^* \)  
time reduced by the travel time in the finger, d

\( t_d \)  
travel time in the distribution zone, d

\( t_f \)  
travel time in the finger, d

\( t_{d+f} \)  
travel time in the distribution zone and the finger, d

\( t_{d+f}' \)  
approximate travel time in the distribution zone and the finger, d

\( v_r \)  
radial flow velocity, m d\(^{-1}\)

\( v_v \)  
vertical flow velocity, m d\(^{-1}\)

\( z \)  
vertical coordinate, positive downwards, m

\( z^* \)  
depth, reduced by the depth of the finger bottom, m

\( a \)  
soil-characteristic constant, m\(^{-1}\)

\( \theta_d \)  
volumetric water content of the distribution zone

\( \theta_f \)  
volumetric water content of the finger

\( \theta_r \)  
residual volumetric water content of the wettable soil

\( \theta_s \)  
saturated volumetric water content of the wettable soil

\( \lambda_n \)  
constant, defined by equation (32)

\( \mu_n \)  
constant, defined by equation (33)

\( \phi \)  
matric flux potential, m\(^2\) d\(^{-1}\)
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APPENDIX A: Flow according to Dupuit in the distribution zone

In the model of the distribution zone presented, the shape of the flow domain is fixed. Hence, the flow is not affected by soil properties other than the water content. If the flow is assumed saturated over a horizontal plane, Dupuit's assumptions can be invoked to incorporate the effect of the saturated hydraulic conductivity on the flow.

Dupuit's assumptions regarding saturated, unconfined flow are (Bear and Verruijt, 1987, pp. 45-52):
- the water flow is parallel to the impermeable base
- the flow velocity is independent of $z$
- the flow velocity is governed by the local gradient of the hydraulic head.

The third assumption gives:

$$q(x) = -2\pi r K_d D_s(x) \frac{dH}{dr}$$  \hspace{1cm} (A1)

For saturated, unconfined flow holds:

$$\frac{dH}{dr} = \frac{dD_s}{dr}$$  \hspace{1cm} (A2)

Incorporating precipitation at the soil surface and drainage into the finger gives:

$$q(x) = -P\pi(R^2-r^2), \quad R_f < r < R$$  \hspace{1cm} (A3a)

and

$$q(x) = -P\pi \left(\frac{R^2}{R_f^2} - 1\right)r^2, \quad 0 < r < R_f$$  \hspace{1cm} (A3b)

Combining equations (A1), (A2), and (A3) gives the differential equations linking $L_r$ to $r$:

$$D_s(x) \frac{dD_s}{dr} = \frac{1}{2} \frac{dD_r^2}{dr} = \frac{P R^2}{2 K_d} r - \frac{P}{2 K_d} r, \quad R_f < r < R$$  \hspace{1cm} (A4a)
These equations can be integrated subject to the conditions that \( L_s \) be zero at \( r = 0 \) and that the \( L_s \) at \( R_f \) calculated from both equations are equal. This gives the following explicit expressions:

\[
D_s(r) \frac{dD_s}{dr} = \frac{1}{2} \frac{dD_s^2}{dr} = \frac{P}{2K_d} \left( \frac{r}{R_f} \right)^2 \ln \left( \frac{r}{R_f} \right), \quad 0 \leq r \leq R_f
\]

(A4b)

\[
D_s = \left[ \frac{PR^2}{K_d} \ln \left( \frac{r}{R_f} \right) + \frac{P}{2K_d} \left( R^2 - r^2 \right) \right]^{\frac{1}{2}}, \quad R_f \leq r \leq R
\]

(A5a)

and

\[
D_s = \left[ \frac{P}{2K_d} \left( \frac{R^2}{R_f^2} - 1 \right) \right]^{\frac{1}{2}} \ln \left( \frac{r}{R_f} \right), \quad 0 \leq r < R_f
\]

(A5b)

The horizontal flow velocity is given by:

\[
v_h(r) = \frac{g(r)}{2\pi r D_s(r) \theta_d}
\]

(A6)

Combining equations (A3), (A5), and (A6) yields the expression for \( v_r \) as a function of \( r \):

\[
v_h = \frac{(2PK_d)^{\frac{1}{2}} \left( R^2 - r^2 \right)}{2\theta_d r \left[ R^2 \ln \left( \frac{r}{R_f^2} \right) + 1 \right]^{\frac{1}{2}}}, \quad R_f \leq r \leq R
\]

(A7a)
and

\[ v_h = -\frac{1}{2\theta_d} \left[ 2PK_d \left( \frac{R^2}{R_f^2} - 1 \right) \right]^{\frac{1}{2}}, \quad 0 < r < R_f \]  

(A7b)

Unfortunately, equation (A7a) cannot be integrated analytically to yield the travel time in the distribution zone. Hence, for flow in the distribution zone according to Dupuit, the analytical approach employed in the main text fails.

However, assigning realistic values to the parameters allows a comparison between the flow velocities calculated by both approaches. The sandy soil near Ouddorp, The Netherlands, exhibits strong water repellency in the top 0.15 to 0.30 m [see also Ritsema et al., 1993]. For this soil layer, \( \theta_d \) at saturation equals 0.5, and \( K_d = 9.6 \text{ m d}^{-1} \) [de Rooij, 1993, unpublished data]. \( P \) is equal to the Dutch mean daily net precipitation, 0.001 m d\(^{-1}\), or ten times this value. Arbitrarily imposing an \( R_f \) of 0.025 m and an \( R \) of 0.50 m results in \( L_d \) equal to 0.0088 m for \( P = 0.001 \text{ m d}^{-1} \), and equal to 0.0279 m for \( P = 0.001 \text{ m d}^{-1} \). These values provide \( L_d \) in equation (1). Figure A1 presents the resulting velocities.

![Figure A1. Radial velocity in the distribution zone according to the model in the main text (equation [1]) and the model in the Appendix (equation[A7]).](image-url)
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