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"Stochastic Simulation of Water Flows in Unsaturated Soil. Comparison with Observed Values"

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STOCHASTIC SIMULATION OF WATER FLOWS IN UNSATURATED SOIL. COMPARISON WITH OBSERVED VALUES

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ABSTRACT

Conceptual modelings of transient water movement in the vadose zone are coupled with a stochastic description of soil properties in order to simulate water flows in spatially variable fields. The heterogeneity of soil properties is described through a single stochastic parameter : the scaling factor.

Solutions are derived for gravity drainage, infiltration at either constant water content or constant flux applied at the surface, and compared with experimental results obtained on a one hectare bare field.

All the results suggest that the use of the traditional deterministic approach is questionable for solving flow equations in case of non homogeneous soils. It is also demonstrated that the concept of effective properties is meaningless for transient flow conditions.

INTRODUCTION

Water infiltration into the vadose zone is a phenomenon of great interest in agricultural and hydrological applications. Until recently, the traditional approach was to consider the field as a homogeneous domain and to apply theories and results valid for laboratory columns. However "large-scale" fields (of the order of a few square meters to tens of square kilometers) display a wide variation of their hydraulic properties (i.e. hydraulic conductivity -water pressure head- water content relationships). Regarding such fields as unique homogeneous columns is highly questionable.

In the last years, systematic field measurements have been performed in order to analyze and to characterize field or watershed spatial variability. This heterogeneity in the soil properties, when coupled with physically-based models yields complex responses through combined stochastic-conceptual modeling.

This paper presents the stochastic-conceptual modeling of the transient infiltration under concentration or flux-type surface conditions in a spatially variable field of which the soil properties are briefly analyzed.

STOCHASTIC-CONCEPTUAL MODELING

The actual field lying in the (x,y) plane is viewed as a collection of uniform and homogeneous vertical columns differing in their hydraulic properties. As a result, water flow due to the application at the surface of a time -and space- independent water content θ_S or water flux q_o will differ from profile to profile. In spite of the field heterogeneity, water movements are considered to be only one-dimensional vertical.

The conceptual model

Under the above assumptions, water flow in each homogeneous column is well-described by the equation :

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D(\theta)\frac{\partial \theta}{\partial z}\right) - \frac{K(\theta)}{\partial z} \qquad (1)$$

subject to the following initial and boundary conditions :

i) - infiltration at constant water content on the surface

$$z \geqslant 0 \qquad t < 0 \qquad \theta = \theta_n \qquad (2a)$$

$$z = 0 \qquad t \geqslant 0 \qquad \theta = \theta_S \qquad (2b)$$

ii) – infiltration at constant flux on the surface

$$
\begin{array}{llll}
z \geq 0 & t < 0 & \theta = \theta_n & \\
z = 0 & 0 \leq t < t_p & -D(\theta)\, \partial\theta/\partial z + K(\theta) = q_o & (3b) \\
z = 0 & t \geq t_p & \theta = \theta_S & (3c)
\end{array}
$$

In these equation, z(m) and t(s) are the depth positively oriented downwards and the time, q_o(ms^{-1}) is the volumetric water flux applied at $z = 0$ which can bee either smaller or greater than the saturated hydraulic conductivity, $K(\theta)$ (ms^{-1}) is the hydraulic conductivity, $D(\theta)$ ($m^2\ s^{-1}$) the soil water diffusivity, θ_n and θ_S are the initial and natural saturated volumetric water contents, respectively, and t_p(s) is the ponding time.

Quasi analytical solution of Eqs (1) and (2) was proposed by PHILIP ([1][2]) and it has been intensively used by many authors.

An approximate quasi-analytical solution of Eqs (1) and (3) can also be obtained by using the flux-ratio concept ([3]) defined as :

$$F(\theta^*, t) = (q - K_n)/(q_S - K_n) \qquad (4)$$

where q_S is the soil surface flux as a function of time and θ^* is the reduced water content :

$$\theta^* = (\theta - \theta_n)/(\theta_o - \theta_n) \qquad (5)$$

θ_o being the time-dependent surface water content. In Eq. (4) K_n stands for $K(\theta_n)$.

It has been shown [4,5] that the time dependence of $F(\theta^*, t)$ was negligible and the corresponding values were well approximated by $F(\theta^*, t) = \theta^*$.

While for a uniform and homogeneous vertical column, $D(\theta)$ and $K(\theta)$ are independent of space, in non uniform fields they vary with x and y. If the soils at sites randomly scattered across a field can be assumed to be similar porous media, then the hydraulic conductivities, soil water-pressure heads and soil water-diffusivities at any site located in the (x,y) plane are given by :

$$K(\theta) = \alpha^2 K^*(\theta) \ ; \ h(\theta) = \frac{1}{\alpha} h^*(\theta) \ ; \ D(\theta) = \alpha D^*(\theta) \qquad (6)$$

where α is a scaling factor describing that particular site ; $K^*(\theta)$, $h^*(\theta)$ and $D^*(\theta)$ are the "scaled mean values" of conductivity, pressure head and capillary diffusivity respectively at a specified water content.

Introducing these relationships into the deterministic quasi-analytical solutions yields :

a) – for infiltration at constant surface water content :

$$z(\theta, t) = \Sigma\, f^*_q(\theta)\, \alpha^{(3q/2-1)}\, t^{q/2} \quad \text{for } t < t^*_c/\alpha^3 \qquad (7a)$$

$$z(\theta, t) = z^*_\infty/\alpha + \alpha^2 u^*(t - t_c) \quad \text{for } t > t^*_c/\alpha^3 \qquad (7b)$$

where f^*_q are the solutions of ordinary differential equations ; t^*_c is the critical time defined as [2] :

$$t^*_c = \left[\frac{A^*_1}{K^*_o - K^*_n}\right]^2$$ where A^*_1 is the "scaled mean" sorptivity and K^*_o is the "scaled mean" conductivity at natural saturation ; z^*_∞ and u^* are the asymptotic profile and translation velocity respectively [2]. More details about these derivations are given in [6].

b) – for infiltration at constant flux

i) – for the non-ponding case ($0 < t < t_p$) the time evolution of the surface water content is given by :

$$[q_o - \alpha^2 K^*_n]^2 = \int_{\theta_n}^{\theta_o} \frac{\alpha[\theta - \theta_n]\, D^*(\theta)}{\theta^* - \alpha^2[K^*(\theta) - K^*_n]/[q_o - \alpha^2 K^*_n]}\, d\theta \qquad (8)$$

and the profile evolution is given by

$$[q_o - \alpha^2 K^*_n]z = \int_{\theta}^{\theta_o} \frac{\alpha\, D^*(\theta)}{\theta^* - \alpha^2[K^*(\theta) - K^*_n]/[q_o - \alpha^2 K^*_n]}\, d\theta \qquad (9)$$

ii) – the ponding time t_p at any location is directly obtained by setting $\theta_o = \theta_S$ in Eq.(8) which is constant over the field as a consequence of the similarity concept.

iii) – for the post-ponding case ($t \geq t_p$), the flux entering through the soil surface is implicitly given by :

$$t - t_p = T(q_S) - T(q_o) \qquad (10)$$

with :

$$T(q) = \frac{1}{[q-\alpha^2 K^*_n]^2} \int_{\theta_n}^{\theta_S} \alpha\{(\theta-\theta_n) D^*(\theta) \left[\frac{1}{\theta^* - \alpha^2 [K^*(\theta) - K^*_n]/[q-\alpha^2 K^*_n]}\right.$$

$$+ \frac{q - \alpha^2 K^*_n}{\alpha^2 [K^*(\theta) - K^*_n]} + \theta^* \frac{[q-\alpha^2 K^*_n]^2}{\alpha^4 [K^*(\theta) - K^*_n]^2} \text{Ln}\left(1 - \alpha^2 \frac{K^*(\theta) - K^*_n}{(q-\alpha^2 K^*_n)\theta^*}\right)]\} \, d\theta$$

and the corresponding water content profile is :

$$[q_S - \alpha^2 K^*_n] z = \int_{\theta}^{\theta_S} \frac{\alpha D^*(\theta)}{\theta^* - \alpha^2 [K^*(\theta) - K^*_n]/[q_S - \alpha^2 K^*_n]} \, d\theta \qquad (11)$$

The runoff rate is then obtained by $R(t,\alpha) = q_o - q_S(t,\alpha)$ (12)
In case of variable initial water content from profile to profile, θ_n and consequently θ^* should be considered as function of α as well, ($\theta_{n,\alpha}$).

All the variables of interest (e.g. moisture profiles, infiltration and runoff rates) are random functions of the single random variable and deterministically depend upon z and t for given deterministic boundary conditions.

Expectation values of the random variates of interest were computed with a weighting average procedure based on RIEMANN-STIELJES integration formulae [7]. It allows a direct evaluation of the statistical first moments of the solution which is much more efficient in terms of computing time than the traditional MONTE CARLO method.

SOIL DATA

The model is applied to a spatially variable field for which the hydraulic properties were obtained from experiments performed on a one-hectare bare sandy soil [6]. Four plots (1.5x1.5m) laterally bounded by a 1.5 m deep plastic sheet were prepared for flood irrigation and subsequent internal drainage. Each plot was equipped with a neutron probe access tube down to 4 m and 10 tensiometers at z = 0.10, 0.20, 0.30, 0.4, 0.5, 0.7, 0.9, 1.10, 1.30 and 1.5 m, connected to mercury manometers. In addition 19 sites were equipped with a neutron probe access tube down to 1.5 m and 3 tensiometers at z = 1.0, 1.1 and 1.20 m. A each site a double ring infiltrometer test was performed in order to analyze the infiltration process and the subsequent drainage. All the 23 sites were located at nodes of a 23 m-square grid.

Neutron readings showed that θ_n and θ_S were very uniform within each observed profile. From profile to profile, they displayed an important variability in θ_n (mean value m = 0.03 m^3/m^3 ; coefficient of variation : CV = 0.58) and great uniformity in θ_S (m = 0.30 m^3/m^3 ; CV = 0.023).

The water contents and hydraulic heads measured on the four plots during the redistribution were analyzed by the instantaneous profiles method in order to obtain the soil hydraulic properties $h(\theta)$ and $K(\theta)$ at several depths. Furthermore, the simultaneous measurements of water content and water pressure head at the three depths on the nineteen sites provided the corresponding $h(\theta)$-curves.

All the $h(\theta)$ and $K(\theta)$ data were scaled [8] through the following "mean scale functions" :

$$K^*(\theta) = K^*_o \left(\frac{\theta}{\theta}\right)^b \quad \text{with} \quad K^*_o = 6.74 \; 10^{-5} \text{ m/s} \qquad (13)$$
$$b = 6.87$$

$$h^*(\theta) = h^*_o \left(\frac{\theta}{\theta_S}\right)^\beta \quad \text{with} \quad h^*_o = -0.166 \text{ m of water} \qquad (14)$$
$$\beta = -1.294$$

The "mean scale" capillary diffusivity function derived from $D^*_o = K^* \frac{dh^*}{d\theta}$ was :

$$D^*(\theta) = D^*_o \left(\frac{\theta}{\theta_S}\right)^{\gamma} \quad \text{with } D^*_o = 4.815\ 10^{-5}\ m^2/s \qquad (15)$$

$$\gamma = 4.576$$

The probability density function of the corresponding scaling factors was found to be log-normal :

$$g(\alpha) = \frac{1}{\sqrt{2\pi}\alpha\sigma_X} \exp\left\{-\frac{(X-m_X)^2}{2\sigma^2_X}\right\} \qquad (16)$$

with $m_X = -0.1229$ and $\sigma^2_X = 0.2782$ where $X = \mathrm{Ln}\ \alpha$.

Furthermore, semi-variograms showed that the scaling factors relating to the $h(\theta)$ observations available at 23 sites and 3 depths were randomly distributed over the field for the considered sampling scheme.

For the 4 plots, the scaling factors obtained from the $K(\theta)$ data were highly linearly correlated (coefficient of determination: 0.85) with the α-values determined from the h( ) data. This implies that the assumption of similar porous media was quite reasonable for the stochastic modeling of the soil hydraulic properties. Furthermore, tensiometer readings at the 23 sites showed that the hydraulic head gradients at z = 110 cm were very close to -1 over a two month-period of measurements. In order to apply our infiltration model with realistic field values of initial water content $\theta_{n,\alpha}$, the water redistribution after saturation of soil profiles has been modeled with the gravity drainage assumption [9].

The corresponding time-evolution of water content at any site characterized by its scaling factor is then given by :

$$\theta(z,t,\alpha) = \theta_S \left\{1 + \alpha^2 \cdot \frac{b-1}{\theta_S} \cdot K^*_o \frac{t}{z}\right\}^{1/1-b} \qquad (17)$$

ILLUSTRATIVE RESULTS

Gravity drainage

The stochastic equation describing the drainage after saturation (Eq. 17) has been solved for z = 110 cm.

The time evolution of $\hat{E}(\theta)$ is given in Fig. 1 as well as the confidence interval at 68 % . Mean values and standard deviation of the 23 measurements are also reported.

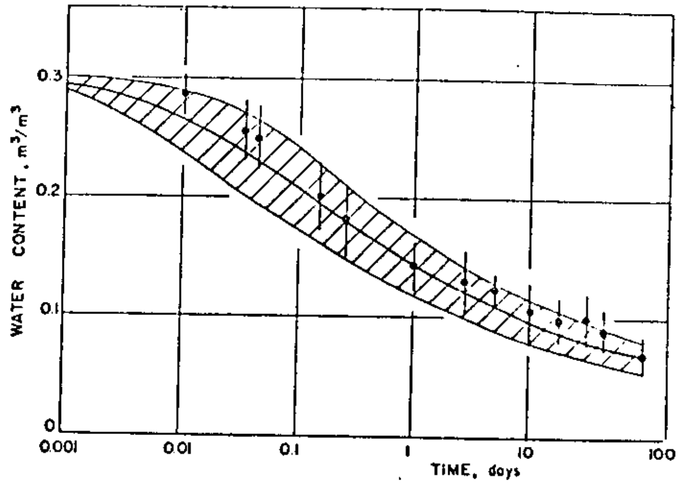

Fig. 1 : Calculated (——) and observed (.) time-evolutions of mean water content at z = 110 cm for drainage. Hatched area corresponds to the calculated 68 % confidence level-vertical bars show the observed standard deviations.

Infiltration at constant surface water content

Solving Eqs (7a) and (7b) for each α_i-value allows to calculate cumulative infiltration $I(t, \alpha_i)$. The time-evolution of $\hat{E}(I)$ is presented in Fig. 2 as well as the deterministic mean $I(m_\alpha)$ obtained by setting $m_\alpha = 1$ (reference soil in the scaling procedure) in Eqs (7a) and (7b). Experimental mean values and range of variation of the 23 measurements are also reported in Fig. 2.

The good agreement between measured and calculated values for these two types of flow tends to show besides the validity of the numerical procedure, that the use of a set of scaling factors as a tool for describing the variability of hydraulic properties is realistic for this soil.

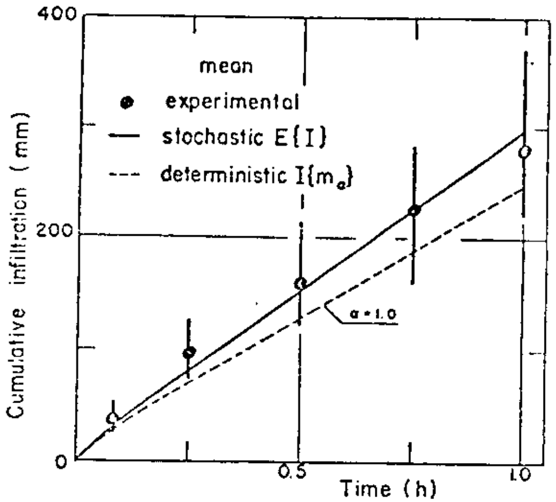

Fig. 2 : Calculated (——) and observed (.) time-evolutions of mean cumulative infiltration. Vertical bars show the range of the observations.

Infiltration at constant flux

As an example of modeling, a total amount of rainfall of 0.121 m has been assumed to take place during different infiltration times (18000, 3600, 1800, 900 and 360s). These values give reduced fluxes $r=q_o/K^*_o$=0.1, 0.5, 1, 2 and 5 respectively. Two kinds of simulation are considered :

i) - random initial condition, RIC which corresponds to variable θ_n, from profile to profile. The calculations have been made by Eq. (17) with t = 10 days.

ii) - Mean initial condition, MIC ; which represents an uniform hypothetical θ_n ($\hat{E}(\theta_{n,\alpha})$= 0.096 m^3/m^3) over the entire field.

The corresponding solutions ($\hat{E}(\theta)$ and σ^2_θ as function of z) are shown in Fig. 3 for three times. The deterministic solutions are also plotted.

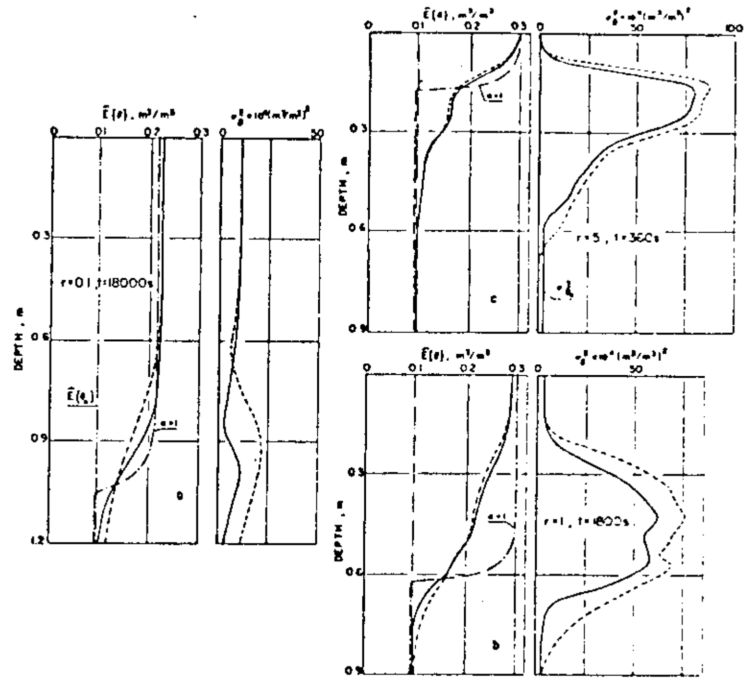

Fig. 3 : Mean and variance water content profiles at three recharge rates ($r=q_o/K^*_o$) for the RIC (——) and MIC (----) simulations. The deterministic simulation corresponds to α = 1.

Table 1 provides the corresponding values of actual mean runoff rate and the cumulative mean runoff, as well as deterministic and potential values. The results clearly demonstrate the differences between the stochastic and deterministic modeling of water infiltration in a variable field.

The deterministic modeling of water movement along soil profile leads to a slight underestimation of the surface water content for small values of q_o (Fig. 3a) and to an overestimation of θ_o for higher values (Figs. 3b,c). The wetting front positions are drastically underestimated whatever the q_o-values are, especially when the runoff becomes significant. The corresponding moisture profiles appear to be much closer to a piston flow shape than those calculated by the stochastic model for which the spreading increases with the recharge rate intensity. Obviously no deterministic runoff can be predicted for fluxes smaller than K^*_o (see Table 1).

r	% Ponded area	Actual mean runoff rate (10^{-6} m/s) $\hat{E}(R)$ RIC	$\hat{E}(R)$ MIC	Deterministic	Potential runoff rate (10^{-6} m/s) R_p	Actual cumulative mean runoff (m) $\hat{E}(CR)$ RIC	$\hat{E}(CR)$ MIC	Deterministic	Potential cumulative runoff (m) (Rp x t)
0.1	2.	.03	.03	0.	.04	.0003	.0002	.0	0.0001
0.5	33.	4.45	4.46	0.	4.91	.0110	.0097	.0	0.0177
1.	5[illegible].	19.67	19.83	0.	21.02	.0282	.0273	.0	0.0378
2.	8[illegible].	67.3[illegible]	67.20	65.30	69.71	.0513	.0511	.039	0.0627
5.	96.	245.5	248.9	266.5	254.1	.0802	.0804	0.069	0.0915

Table 1 - Comparison between deterministic, stochastic and potential values of mean runoff rate and cumulative mean runoff for 5 reduced fluxes.

$$R_p = \frac{q_o}{2} \left| 1 + \mathrm{erf}\left(\frac{\frac{1}{2}\,\mathrm{Ln}\, r - m_X}{\sqrt{2}\,\sigma_X}\right) - \frac{1}{r}\exp(2\sigma_X^2 + 2\,m_X)\left(1 + \mathrm{erf}\left(\frac{\frac{1}{2}\,\mathrm{Ln}\, r - (m_X + 2\sigma_X^2)}{\sqrt{2}\,\sigma_X}\right)\right)\right|$$

Although for r=2, the runoff rate is underestimated by the deterministic approach, for r = 5 it becomes overestimated and greater than the potential rate value itself. This behaviour can be partly explained by means of Fig. 4 where R_p/q_o is given as a function of q_o/K^*_o for both the deterministic ($R_p/q_o = 1-1/r$) and stochastic approaches. In addition the values of $\hat{E}(R)/q_o$ for the RIC simulation (Table 1) are also reported. From this figure it clearly appears that for r = 2.2, the potential runoff which would be predicted by the deterministic modeling becomes higher than that obtained by the stochastic one, for the observed soil variability.

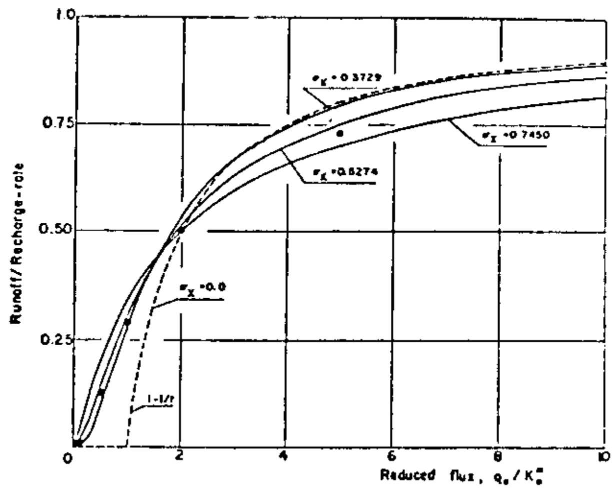

Fig. 4 : Runoff to recharge rate ratio as function of reduced flux. Dashed line is the deterministic relation. Continuous lines are the potential values (see Table 1) for 3 standard deviations of X = Ln α. Black points are the actual values.

In addition, the following remarks are suggested :

i) - For a given rainfall intensity, the RIC- or MIC- types have little influence on the stochastic mean profiles, except may be near the wetting fronts (Figs. 3) and on the actual mean runoff values as well (Table 1). On the other hand, taking into account variable initial condition tends to reduce moisture profiles variability.

ii) - For higher values of the recharge rate intensity, the variances become smaller close to the surface since the steady state regime prevails quicker and maximum variances are greater. Note that considering either RIC- or MIC simulations or doubling the intensity have approximatively the same effect on the value of this maximum.

iii) - Fig. 4 shows that the runoff is an increasing function of soil variability for small values of q_o. For high recharge rates, field heterogeneity tends to reduce R_p/q_o making thus the deterministic approach more and more questionable.

Effective properties

If the required information about the flow is restricted to average values $<\theta>$, one may seek to define an equivalent homogeneous soil such that the solution of the flow problem (Eqs 1 to 3) in this medium, is identical to the average values of the heterogeneous field. For such a soil, its properties are called "effective" properties. They would be defined by :

$$<K> = -<q>/(d<h>/dz-1) \quad (18)$$

$$<h> = h\ (<\theta>) \quad (19)$$

Then the general flow equation (Eq. 1) becomes :

$$\frac{\partial<\theta>}{\partial t} = \frac{\partial}{\partial z}\left(<D> . \frac{\partial<\theta>}{\partial z}\right) - \frac{\partial<K>}{\partial z}$$

where the effective diffusivity is given by $<D> = <K> . \frac{d<h>}{d<\theta>}$.

If $<K>$, $<h>$ and $<D>$ do exist solving Eq. 19 for a variable field is similar to the traditional deterministic approach.

As an example, Fig. 5 present the relationships between $<K>$, $<h>$ and $<\theta>$ calculated by solving Eqs. 8 to 11 for different values of q_o. The initial water content is $\hat{E}(\theta_n) = 0.096\ m^3/m^3$. The results clearly demonstrate that effective properties defined by the equations (18) depend on the flux applied at the surface. Other calculations not presented here show that they also depend on initial water content. Also are plotted in these figures, the effective properties corresponding to steady-state infiltration regime when $q_o \to 0$ and $q_o \to \infty$. In the former case the effective conductivity at saturation $<K>_S$ is the geometrical mean. In the latter one, it corresponds to the arithmetic average.

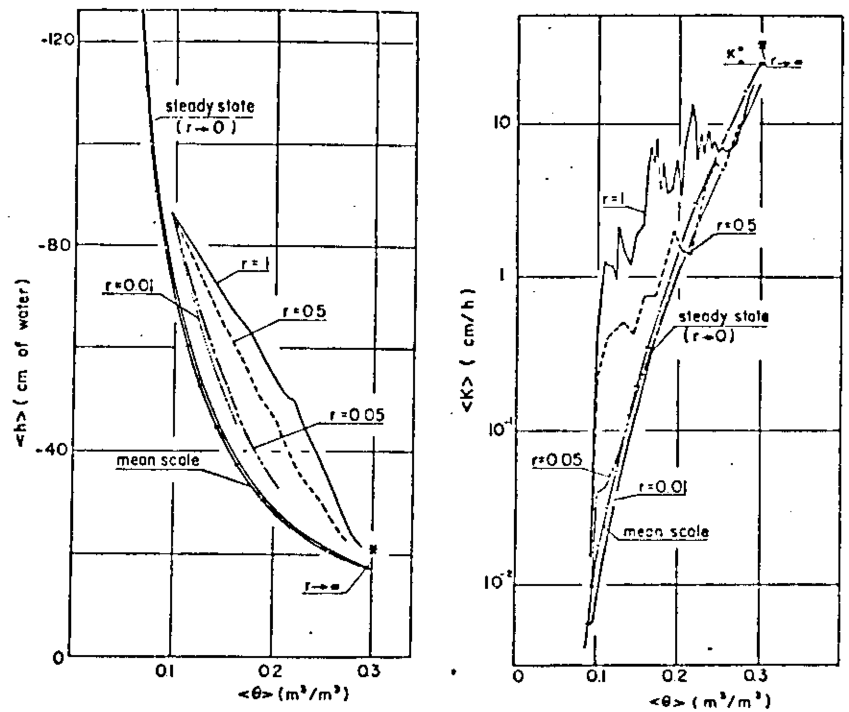

Fig. 5 : Effective hydraulic properties (Eqs 18).

Hence, for this particular flow regime, one can obtain mean values in an equivalent homogeneous soil by taking $<K>_S$ varying between geometrical (non ponding) and arithmetic (flooding) means and air entry value close to h^*_o (Fig. 5).

For transient flow regimes it appears that effective properties are meaningless. Considering any flow equation (FOKKER-PLANCK, RICHARDS) associated with the concept of equivalent uniform soil does not seem to be valid to simulate water movements in heterogeneous fields.

These findings are very similar to those reported by |10,11| and obtained by other methods of calculations based on different physical assumptions.

CONCLUSION

The results presented here show that a physically-based model of water flow in the vadose zone coupled with a stochastic description of the soil hydraulic properties yields very realistic responses of a spatially variable field. The traditional deterministic approach cannot be justified in solving flow equations in case of heterogeneous fields mainly because the effective properties concept seems to be meaningless.

REFERENCES

[1] PHILIP, J.R. : The theory of infiltration. 1 – The infiltration equation and its solution.
Soil Sci. 83, 1957, pp. 345-357.

[2] PHILIP, J.R. : Theory of infiltration.
Adv. Hydrosc., Academic Press, 1969, pp. 215-305

[3] PHILIP, J.R. : On solving the unsaturated flow equation. 1 – The flux concentration relation.
Soil Sci. 116, 1973, pp. 328-335.

[4] PERROUX, K.M., D.E. SMILES & I. WHITE : Water movement in uniform soils during constant-flux infiltration.
Soil Sci. Soc. Am. J., 45, 1981, pp. 237-240.

[5] BOULIER, J.F., J. TOUMA & M. VAUCLIN : Flux concentration relation-based solution of constant flux infiltration equation. I – Infiltration into non uniform initial moisture profiles.
Soil Sci. Soc. Am. J., 48, 1984, pp. 245-251.

[6] VAUCLIN, M., J. IMBERNON, G. VACHAUD & C. DANCETTE : Description expérimentale et modélisation stochastique des transferts par mise en facteur d'échelle des propriétés hydrodynamiques des sols.
Proceedings of IAEA Symposium Aix en Provence (France), 1983, pp. [illegible].

[7] CRAMER, H. : Mathematical methods of statistic. Princeton University Press, 1961, pp. 575.

[8] SIMMONS, C.S., D.R. NIELSEN and J.W. BIGGAR : Scaling of field-measured soil-water properties. 1 – Methodology. 2 – Hydraulic conductivity and flux.
Hilgardia 47 (4), 1979, pp. 77-173.

[9] LIBARDI, P.L., K. REICHARDT, D.R. NIELSEN & J.W. BIGGAR : Simple field methods for estimating soil hydraulic conductivity.
Soil Sc. Soc. Am. J. 44, 1980, pp. 3-8.

[10] BRESLER, E. & G. DAGAN : Unsaturated flow in spatially variable fields. 2 – Application of water flow models to various fields.
Water Resour. Res. 19, 1983, pp. 421-418.

[11] YEH, T.C., L.W. GELHAR & A.L. GUTJAHR : Stochastic analysis fo effects of spatial variability on unsaturated flow.
Report n° H-11. New Mexico Institute of Mining and Technology.