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THE USE OF SIMULATION MODELS IN THE STUDY OF SOIL MOISTURE TRANSPORT PROCESSES

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ABSTRACT

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The development of high speed computers in recent years, along with the availability of sophisticated simulation languages facilitate the use of computer models in the study of transport processes in soils.

It is shown that a model of evaporation from the soil surface yields satisfactory results and special difficulties encountered during its development and operation are discussed.

Special attention is paid to the hierarchical approach in model building as a means of overcoming problems of multilevel models as well as those of very costly and time consuming execution of detailed models.

It is concluded that simulation models are a strong tool in the study of transport processes in the soil, not only in solving specific problems but also in pinpointing to weak areas in our knowledge and hence to the design of new experiments.

INTRODUCTION

Transport processes in the rather complicated porous soil system play an important role in many disciplines. Agronomists are dealing with them because they govern processes of plant growth by supplying the necessary water and minerals to the plant root. In more recent years, specially water management engineers, responsible for the continuous supply of good quality water for human consumption and agricultural purposes are interested in the behaviour of the soil water, and those concerned with problems of pollution are forced to predict the fate of solutes landed in the soil on purpose or accidentally.

The transport processes are characterized by a simultaneous change in the amount of material with time and place. In mathematics such distributive systems are described by partial differential equations. Analytical solutions for these equations can in general only be found for problems that are so simple, that they are only of academic interest, or under greatly simplifying assumptions making the conclusions arrived at of little practical value. Where the analytical solutions fail to provide an answer, the brute force of the computer may help to solve the problem.

The development of sophisticated simulation languages containing features to overcome the main disadvantages of digital calculation machines, which contrary to natural systems operate discontinuously and sequentially, has facilitated the use of these machines. Moreover these languages easily handle problems of numerical integration, providing a number of methods each with its own advantages in specific situations.

The application of one of these languages, the Continuous System Modeling Program (CSMP), developed by IBM for its 360 and 370 series of machines for the

development of simulation models for transport processes in the soil has been demonstrated by De Wit & Van Keulen (1972). In this paper a model for soil evaporation is described and a technique to use such models in plant productivity studies is proposed.

THE EVAPORATION MODEL

Evaporation from the soil surface is one of the main causes of nonproductive water loss under conditions where the atmospheric demand is high (arid and semi-arid regions) and the soil is not or only sparsely covered for prolonged periods of time. To estimate the amount of water available for plant growth, it is of primary importance to be able to predict the evaporative losses. For this purpose a simulation model was developed that calculates the evaporative flux from a bare soil surface from meteorological data and from physical properties of the soil. A detailed description of this model is presented elsewhere (Van Keulen, 1974).

Based on the principles of the finite difference method, as pointed out by De Wit & van Keulen (1972), the simultaneous flow of heat and water in a soil column is calculated.

Moisture is transported either in liquid form under a potential gradient or in the vapor phase under a gradient of vapor pressure, taking into account the appropriate transport coefficients.

Heat is transported by diffusion along a temperature gradient and by mass transport along with the flow of water.

The surface temperature is calculated from the energy balance at the soil surface: absorbed short wave radiation, sensible heat loss, outgoing long wave radiation, heat flow into or out of the soil and evaporative heat loss.

The evaporative heat loss is obtained from the difference in vapor pressure between the soil surface and the atmosphere and the aerodynamic resistance for vapor transport above the soil surface. The aerodynamic resistance is calculated from the wind speed, taking into account the roughness height of the surface elements, according to a semi-empirical formula developed by Chamberlain (1968). The vapor pressure at the soil surface is obtained from the surface temperature, taking into account the vapor pressure depression due to increasing soil moisture potential.

Sensible heat loss is calculated from the temperature difference between the soil surface and the atmosphere and the resistance for heat exchange, the latter being proportional to the vapor exchange coefficient. Outgoing long wave radiation is estimated with an empirical formula given by Brunt (1932). Soil heat flux is calculated from the difference in temperature between the soil surface and the middle of the first, 1 cm thick, compartment, and the moisture content dependent heat conductivity of the soil.

In figure 1 the measured and calculated cumulative evaporation of a uniform löss column under laboratory conditions is given, while in fig. 2, the measured (γ -ray attenuation) and calculated soil moisture profiles are compared. The agreement in the cumulative evaporation is excellent, the moisture profiles however show deviations. This may be attributed to disturbances in the soil column, as the drying of the soil caused shrinkage, leading to cracks at the soil surface and to the development of air spaces at some points along the perspex walls. These disturbances presumably caused changes in the hydraulic properties of the soil, while in the simulation program constant K- Θ and Ψ - Θ relations are used. Moreover these relations were determined in duplicate columns, which may not have been completely identical, thus causing different hydraulic properties too.



 $\underline{Fig.~l}.$ Comparison between measured and simulated cumulative evaporation from a uniform column of löss.



<u>Fig. 2</u>. Measured (a) and simulated (b) soil moisture profiles in a uniform löss column under constant evaporative conditions. Numbers along the graph indicate days after the start of the experiment.

It may be concluded however that the present model gives satisfactory results in predicting the evaporative water loss from a bare soil surface. This is supported by the results shown in figure 3, where the same model has been applied to a field situation.



The determination of the physical parameters of the soil, specially under field conditions, is still one of the biggest problems in the modeling approach. Although it is possible to test the validity of a model under laboratory conditions and to estimate the physical properties from a given field by successive trial and error through comparison with actual field data, this procedure remains unsatisfactory as one is never sure that not a difference in response of the system between field and laboratory occurs. It seems to me therefore of the greatest importance, that the methods to determine the physical properties of soils in situ are improved.

THE APPLICATION OF SOIL MOISTURE TRANSPORT MODELS

Apart from gaining more insight into the relevant processes, which is one of the purposes for the development of simulation models, in our case the main aim is the application of such models to predict the availability of water for plant growth.

It turns out however, that, while the periods of interest for plant production are in the order of a hundred days, the time constant of the soil water

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system is in the order of minutes or even seconds due to the explicit method of integration. To simulate such systems, one has to proceed in time with intervals that are in the same order as the time constant of the system. It is obvious, that computer time and budget will soon become the limiting factors for the application of such models. It is therefore necessary to introduce a different approach in the description of soil moisture flow in models that are mainly aimed at the calculation of crop production.

For the process of infiltration a simplification is introduced in which the water entering the soil is divided over the soil compartments from the top one, each one successively filling up to field capacity till all the water is dissipated or till the remainder has drained below the maximum rooted depth.



Fig. 4. Comparison of the moisture distribution after ilfiltration calculated with the simulation model and with the "simplified" method.

In figure 4 a comparison is shown of the moisture distribution in an initially dry soil profile after a rain of 18 mm, calculated with the simplified model and with the simulation model (Van Keulen & Van Beek, 1971; Stroosnijder et al., 1972). It shows that after one day about 95% of the water is in the same soil zone in both cases, while the differences in actual moisture content at various depths will hardly influence the availability to the roots. Under various conditions, the results may deviate somewhat, leading to differences of about 25% in storage in the same soil zone. It is emphasized however that a different situation exists when so much irrigation water is applied that the storage capacity of the soil, i.e. the amount that can be stored in the potential root zone, is highly exceeded. Under perma-dry conditions which exist in most of the arid and semi-arid zones, this schematisation gives satisfactory results. Such simplifications should however always be compared with the results of models based on physical laws.

To describe the process of evaporation from the soil surface in a simple way, a "mimicking" procedure has been developed. The term "mimicking" is used here to define a procedure in which the response of the system to a given set of external conditions is obtained by a special programming or calculation scheme, which in

itself has no physical or physiological meaning. Such a "black box" may also be constructed in situations where the causal relations are not known (Jansen, 1974).

To obtain the evaporation, first the potential evaporation is calculated with the formula of Penman (1956), which gives good agreement with the calculated soil evaporation as shown in figure 3. The actual rate of evaporation is then determined by the moisture potential at the soil surface. Because redistribution of the water between soil compartments as a result of developing potential gradients is omitted in the crop growth model, the total evaporative water loss must be divided over the various compartments. For each compartment the rate of water extraction is written as:

$$\begin{split} & E_{\mathbf{x}} = F \, \bigstar \, \text{AEVAP} \\ \text{with } F = (\bigcirc -\circlearrowright_1) \, \bigstar \, e^{(-P \bigstar d)} \\ & \text{ in which } \circlearrowright \ \ = \text{ actual water content in compartment} \\ & \circlearrowright_1 = \text{ water content at air dryness} \\ & P^1 = \text{ proportionality factor} \\ & d = \text{ depth of centre of compartment below soil surface} \end{split}$$



Fig. 5. Comparison of the moisture distribution and the cumulative evaporation, calculated with the simulation model and with the "mimicking" procedure.

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In figure 5 a comparison is shown between the results of the simulation model and the "mimicking" procedure, in which for P the value 15 was used. It is obvious that this value depends on the moisture transmission properties of the soil under consideration. As the relation between the two depends both on the actual value of the conductivity and on the shape of the K-O relationship no attempt is made to give a general formula, but it is proposed to calculate the value of P by comparison of the simulation model with the "mimicking" procedure for each soil.

CONCLUSION

From the foregoing it is concluded that simulation models are a strong tool in the prediction of the behaviour of soil moisture under varying conditions. A serious disadvantage is however the very small time constant of the soil moisture system, which limits their use in general to short term processes, although simplifications may be introduced on basis of the results obtained with the simulation models.

The determination of the soil physical parameters in situ should get proper attention to improve the applicability of the simulation models.

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DISCUSSION

It seems to me that you take great pride in being as precise as possible in doing the modeling and you then are extremely loose when you start using words as better, best, good. You never tell us what you mean by these statements. Another point is, you made a statement which I think is extremely dangerous, you said, if you did not get an agreement you went back and you put in more detail. That's not necessarily a good way of getting a better agreement. (YOUNG)

I did not specify good, better, best due to lack of time. The second one, I think you probably misunderstood : the point is not that putting in more detail should give you any better result à priori but the point is that, when you have described a process with a number of equations which you think are representing the process and you don't get agreement between the observed and the calculated results you should go back to your set of mathematical equations, study them again and see if you did not leave anything out. (VAN KEULEN)

I might say there is a very close analogy between your material energy balance use and the one that we did on the rivers where we look at the evaporative enthalpy loss of heated water to the atmosphere. Do you have an evaporative enthalpy loss term ? (DAVIDSON)

No. (VAN KEULEN)

We found that in the river the evaporative enthalpy loss term is roughly 50 % of the heat loss when you look at the long way, the short way, the force conduction and then look at the evaporative enthalpy loss term itself, which is a large quantity. I suspect you have to look at it. The second question has to do with the time base for input data in your heat exchange formulas. We found that using daily average versus data based say on hourly readings, you can pick up another 30 to 40 % deviation between the cumutative effects and those which are actually accumulating on your integral or shorter time history. The heat exchange factors change enormously over a cycle of 24 hours. (DAVIDSON)

Yes, when possible we use weather data on the smallest base that is available, that means on the base of the calculation. In many cases you don't have them. We have developed some procedures which convert daily averages back into daily courses. (VAN KEULEN)

You mentioned that you have very small timesteps like minutes, I was wondering whether this would not be a direct consequence of using CSMP which I understand is quite an explicit procedure. Using evaporation data like we did, we could use timesteps of a day or more. (NEUMAN)

In the runoff model where we use evaporation, I use timesteps of a day with this limiting procedure, I got satisfactory results. (VAN KEULEN)

What kind of integrator do you use ? (TODINI)

Either Runge Kutta or Milne with variable timesteps. (VAN KEULEN)

You can have larger timesteps. (TODINI)

I agree with that. (VAN KEULEN)