Modelling Water Flow and Solute Transport for Horticultural and Environmental Management

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Abstract

During the past 10 years, the simulation model SWAP (Soil, Water, Atmosphere, Plant) was developed by the Sub-Department Water Resources of Wageningen University jointly with the Department Water and Environment of Alterra Green World Research. SWAP simulates vertical transport of water, solutes and heat in variably saturated, cultivated soils at field scale level and during whole growing seasons. Different versions of the model have been applied worldwide in research, education and as a decision support tool in the management of agricultural, horticultural and natural systems water flow in homogeneous and heterogeneous soils with or without the influence of groundwater. The main features of and theoretical concepts behind SWAP are described, in particular soil water flow, solute transport and crop growth.

INTRODUCTION

In the soil numerous interactions occur between water flow, solute transport, heat flow and plant growth. For instance, water fluxes affect the rate of salinization, while salt concentrations affect actual root water uptake rate. Water and salinity stress may affect crop development and soil cover, which vice versa affects soil evaporation and crop transpiration. Pesticide decomposition is sensitive to soil temperatures, which on their turn are influenced by soil wetness. In order to analyse these kind of interactions, SWAP solves simultaneously the numerical equations for water flow, solute transport, heat flow and crop growth, and allows interaction at time step basis (Dam van, et al., 1997; Dam van, 2000).

At the farmer field scale, the meteorological conditions, cultivation pattern, soil profile and drainage conditions are more or less the same and well defined. The input data can be measured directly in the field, or derived from data banks with geographical information. Another important advantage is that such models can be employed for scenario analysis covering a wide range of situations.

In most applications, we are not only interested in the systems behaviour in a particular or ‘average’ meteorological year, but also in its behaviour during extreme weather periods. Furthermore some processes, like salinization and groundwater recharge, require analysis over a large number of years. Therefore long term simulations, without losing accuracy during rapidly changing conditions, constituted one of the main demands.

The model should assist researchers in analysis of field experiments, in testing alternative theoretical concepts and in exploration of all kind of scenarios. Also the model should be useful to students to illustrate the interaction between the various processes and provide quantitative information on their relative importance. Furthermore, the model should be useful to engineers who face daily agrohydrological problems. A basic knowledge of agrohydrological processes however, is essential for proper model use and result interpretation.

Figure 1 schematizes the hydrological processes incorporated in SWAP. The upper boundary is located just above the vegetation, the lower boundary in the top groundwater system. In the region between these boundaries, the main water flow processes are vertical, which allows for a one-dimensional model structure. When a region is analyzed with horizontal variation of vegetation, soil or drainage conditions, the
model should be applied either at each location separately, or a more or less representative situation should be defined. The SWAP soil column is divided in compartments, for which the transport and balance equations of water, solutes and heat are solved. Interaction between residence and movement of water, solute and heat occurs at each time step, which may range between seconds and hours, depending on how fast flow and transport conditions change in time. Interaction with plant growth processes which show relatively slow changes in time, is calculated on a daily basis. SWAP makes a distinction between soil evaporation and plant transpiration, because both have clearly different extraction and reduction mechanisms. In the saturated zone, interaction with water management in canals/ditches at different levels may be calculated. At the bottom of the SWAP column, interaction with regional groundwater is defined. Soil heterogeneity is taken into account by providing options for soil layering, similar media scaling, water repellency and shrinkage cracks.

In the next sections the various elements are described in more detail, starting with water, going from atmosphere to bottom boundary, then solutes, and ending with the user interface.

**POTENTIAL EVAPOTRANSPIRATION**

The upper boundary conditions are determined by the rates of potential evapotranspiration $ET_p$, irrigation and precipitation. Daily meteorological data consisting of air temperature, solar radiation, wind speed and air humidity, can be used to calculate daily potential evapotranspiration according to Penman-Monteith (e.g. Smith, 1992; Allen et al., 1998). If basic meteorological data are not available, potential evapotranspiration rate or reference evapotranspiration rate in combination with crop factors can be input (e.g. Allen et al., 1998). Precipitation may be provided either at a daily basis or at actual intensities. In case of runoff and preferential flow simulation, actual rainfall intensities increase the reliability of the simulation results.

**IRRIGATION**

Irrigation may be prescribed at fixed times or scheduled according to a number of criteria, which allows for the optimization of irrigation management. The timing criteria include allowable daily stress (as expressed by the reduction of potential crop transpiration), allowable depletion of readily available water in the root zone, allowable depletion of totally available water in the root zone and critical soil water pressure head or soil water content at a certain depth. The irrigation amounts can be prescribed or can be calculated by SWAP as the difference between actual water storage in the root zone and water storage at field capacity. The calculated irrigation amounts can be increased to induce leaching, or decreased to account for expected rainfall.

**CROP GROWTH**

SWAP may simulate up to three rotating crops in a year and contains three crop growth routines: a detailed model (WOFOST 6.0; Spitters et al., 1989), the same model but attuned to simulate grass growth only, and a simple model. Figure 2 schematizes the processes incorporated in WOFOST. The program calculates the radiation energy absorbed by the canopy as function of incoming photosynthetic active radiation and crop leaf area. Using the absorbed radiation and taking into account photosynthetic leaf characteristics, the potential photosynthesis rate is calculated. The latter is reduced due to water and/or salinity stress, as quantified by the relative transpiration rate, and yields the actual photosynthesis rate. Part of the carbohydrates (CH$_2$O) produced are used to provide energy for the maintenance of living biomass (maintenance respiration). The remaining carbohydrates are converted into structural matter. In this conversion, some of the weight is lost as growth respiration. The dry matter produced is partitioned among roots, leaves, stems and storage organs, using partitioning factors that are a function of the crop phenological development stage. The fraction partitioned to the leaves, determines leaf
area development and hence the dynamics of light interception. The dry weights of the plant organs are obtained by integrating their growth rates over time. During crop development part of the living biomass will die due to senescence.

In case crop growth does not need to be simulated or when crop growth data are insufficient, the simple crop development model can be used. For this model the user prescribes the leaf area index (or soil cover fraction), crop height and rooting depth as functions of crop development stage, which either is controlled by temperature or is linear in time.

**POTENTIAL SOIL EVAPORATION AND PLANT TRANSPIRATION**

The potential evaporation rate \( E_p \) (cm d\(^{-1}\)) of a soil under a standing crop that partially covers the soil, is derived from the Penman-Monteith equation by neglecting the aerodynamic term. The aerodynamic term will be small because the wind velocity near the soil surface is relatively small, which makes the aerodynamic resistance very large. In case the leaf area index as function of crop development stage is unknown, the fraction of soil cover, \( SC (-) \) might be used to determine \( E_p \):

\[
E_p = (1 - SC) ET_p
\]  
(1)

Based on energy considerations, and after applying a correction for evaporation of intercepted rain or sprinkled water, the potential transpiration rate, \( T_p \) (cm d\(^{-1}\)), equals the potential evapotranspiration rate \( ET_p \) minus \( E_p \):

\[
T_p = ET_p - E_p \quad \text{with} \quad T_p \geq 0
\]  
(2)

**ACTUAL SOIL EVAPORATION**

In case of a wet soil, soil evaporation is determined by the atmospheric demand and equals potential soil evaporation rate \( E_p \). When the soil becomes more dry, the soil hydraulic conductivity \( K \) decreases, reducing \( E_p \) to a lower actual evaporation rate, \( E_a \) (cm d\(^{-1}\)). In SWAP the maximum evaporation rate which the top soil may deliver, \( E_{\text{max}} \) (cm d\(^{-1}\)), is calculated according to Darcy’s law (see also Eq. 6):

\[
E_{\text{max}} = K_{\frac{1}{2}} \left( \frac{h_{\text{atm}} - h_1 - z_1}{z_1} \right)
\]  
(3)

where \( K_{\frac{1}{2}} \) is the average hydraulic conductivity (cm d\(^{-1}\)) between the soil surface and the first node, \( h_{\text{atm}} \) is the soil water pressure head (cm) in equilibrium with the air relative humidity, \( h_1 \) is the soil water pressure head (cm) of the first node, and \( z_1 \) is the soil depth (cm) at the first node. Note that the value of \( E_{\text{max}} \) in Eq. 3 depends on the thickness of the top soil compartments. Increase of compartment thickness, generally results in smaller values for \( E_{\text{max}} \) due to smaller hydraulic head gradients. For accurate simulations at extreme hydrological conditions, the thickness of the top compartments should not be more than 1 cm (Dam van, and Feddes, 2000).

Also empirical evaporation functions may be used, which require calibration of their parameters for the local climate, soil, cultivation and drainage situation. SWAP has the option to choose the empirical evaporation functions of Black et al. (1969) or Boesten and Stroosnijder (1986). SWAP will determine \( E_a \) by taking the minimum value of \( E_p \), \( E_{\text{max}} \) and, if selected by the user, one of the empirical functions.

**ACTUAL PLANT TRANSPIRATION**

The maximum possible root water extraction rate, integrated over the rooting depth, is equal to the potential transpiration rate, \( T_p \) (cm d\(^{-1}\)), which is governed by atmospheric conditions as discussed before. The potential root water extraction rate at a certain depth, \( S_p(z) \) (d\(^{-1}\)), may be determined by the root length density, \( \pi_{\text{root}}(z) \) (cm cm\(^{-3}\)), at this depth as fraction of the total root length density over the rooting depth \( D_{\text{root}} \) (cm) (e.g. Bouten,
Stresses due to dry or wet conditions and/or high salinity concentrations may reduce $S_p(z)$. The water stress in SWAP is described by the function proposed by Feddes et al. (1978), which is depicted in Figure 3. For salinity stress the response function of Maas and Hoffman (1977) is used (Figure 4), as this function has been calibrated for many crops (Maas, 1990). In order to simplify parameter calibration and use of existing experimental data, we assume in SWAP the water and salinity stress to be multiplicative. This means that the actual root water flux density, $S_a(z)$ (d$^{-1}$), is calculated from:

$$S_a(z) = \alpha_w S_p(z)$$

where $\alpha_w$ (-) and $\alpha_s$ (-) are the reduction factors due to water and salinity stresses, respectively. Integration of $S_a(z)$ over the rooting depth yields the actual transpiration rate $T_a$.

**SOIL WATER FLOW**

Spatial differences of the soil water hydraulic head cause flow of soil water. Darcy’s equation is used to quantify these soil water fluxes, which for one-dimensional vertical flow can be written as:

$$q = -K(h) \frac{\partial (h+z)}{\partial z}$$

where $q$ is soil water flux density (positive upward) (cm d$^{-1}$), $K$ is hydraulic conductivity (cm d$^{-1}$), $h$ is soil water pressure head (cm) and $z$ is the vertical coordinate (cm) taken positively upward. Water balance considerations of an infinitely small soil volume result in the continuity equation for soil water:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} - S_a(z)$$

where $\theta$ is the volumetric water content (cm$^3$ cm$^{-3}$), $t$ is the time (d) and $S_a$ is the actual soil water extraction rate by plant roots (cm$^3$ cm$^{-3}$ d$^{-1}$). Combination of Eq. 6 and 7 results in the well-known Richards’ equation:

$$\frac{\partial \theta}{\partial t} = C(h) \frac{\partial h}{\partial t} = \frac{1}{C(h)} \left[ K(h) \left( \frac{\partial h}{\partial z} + 1 \right) \right] - S_a(z)$$

where $C$ is the differential water capacity (d$\theta$/d$h$) (cm$^{-1}$).

Richards’ equation has a clear physical basis at a scale where the soil can be considered to be a continuum of soil, air and water. This physical basis allows the use of generally available soil physical data and the simulation of a wide range of management scenario’s. SWAP solves Eq. 8 numerically in an implicit backward finite difference scheme (Dam van, 2000, see Appendix B) subject to specified initial and boundary conditions and soil hydraulic functions, which relate $\theta$, $h$ and $K$.

**DRAINAGE**

In the saturated part of the soil column, a distinction is made between a drainage and a bottom flux (Figure 5). The drainage flux refers to the groundwater flux to/from the local drainage system. The bottom flux refers to the water flux at the soil profile bottom, which in general is caused by regional groundwater flow. In many other soil water flow
models the drainage flux and bottom flux are combined into the bottom flux. SWAP can be used in the same way, by omitting the drainage component. The feature of defining the local drainage flux separately, allows for simulation of the interaction between surface water management and groundwater levels, the evaluation of drainage alternatives and the residence time of solutes in the saturated zone.

One method to calculate the drainage flux density \( q_{\text{drain}} \) (cm d\(^{-1}\)) is assuming a linear relation between groundwater level \( \phi_{\text{gwl}} \) (cm) and \( q_{\text{drain}} \):

\[
q_{\text{drain}} = \frac{\phi_{\text{gwl}} - \phi_{\text{drain}}}{\gamma_{\text{drain}}}
\]

(9)

where \( \phi_{\text{drain}} \) is the drain level (cm) and \( \gamma_{\text{drain}} \) is the drainage resistance (d).

**BOTTOM BOUNDARY CONDITION**

The following options are offered to prescribe the bottom boundary condition:
- specify the groundwater level or soil water pressure head as function of time;
- specify the bottom flux as function of time;
- specify the bottom flux as function of groundwater level.

Measurements of groundwater levels are relatively easily done and often used during model calibration with experimental data. However, when alternative scenario’s have to be simulated, in most cases the groundwater levels will change, and therefore can not be prescribed anymore. Prescribed bottom fluxes are attractive, as fixed bottom fluxes may increase the accuracy of simulated soil moisture profiles and solute leaching. Unfortunately, efforts to develop reliable and practical instruments to measure soil water fluxes in situ, failed until now. Situations in which the bottom flux can be prescribed occur when a soil layer with a low permeability is present in the subsoil, or when the seepage flux is more or less constant and known. When the groundwater level is relatively deep, we may assume a zero gradient of the soil water pressure head at the bottom of the soil profile, so called free drainage. Application of Darcy’s law gives for such a case:

\[
q = -K(h) \left( \frac{\partial h}{\partial z} + 1 \right) = -K(h)(0 + 1) = -K(h)
\]

(10)

**SOLUTE TRANSPORT**

**Transport Processes**

The three main solute transport mechanisms in soil water are diffusion, convection and dispersion. Diffusion is solute transport which is caused solely by a solute gradient. The solute flux density \( J_{\text{dif}} \) (g cm\(^{-2}\) d\(^{-1}\)) is generally described by Fick’s first law:

\[
J_{\text{dif}} = -\theta D_{\text{dif}} \frac{\partial c}{\partial z}
\]

(11)

where \( D_{\text{dif}} \) is the diffusion coefficient (cm\(^2\) d\(^{-1}\)) and \( c \) is the solute concentration (g cm\(^{-3}\)) in soil water.

The bulk transport of solutes occurs when solutes are carried along with the moving soil water. The mean flux of this transport is called the convective flux density, \( J_{\text{con}} \) (g cm\(^{-2}\) d\(^{-1}\)) and can be calculated from the average soil water flux density \( q \):

\[
J_{\text{con}} = q c
\]

(12)

When describing water flow, we usually consider only the Darcy flux \( q \) (cm d\(^{-1}\)), which is averaged over a certain cross section. In case of solute transport, we need to consider as well the water velocity variation between pores of different size and geometry and also the water velocity variation inside a pore itself. The variety of water velocities causes some solutes to advance faster than the average solute front and other solutes
slower. The overall effect will be that steep solute fronts tend to smoothen or to disperse. Similar to diffusion, solutes seem to flow from high to low concentrations. If the time required for solutes to mix in the transverse direction is small, compared to the time required for solutes to move in the flow direction by mean convection, the dispersion flux density $J_{\text{dis}} \ (\text{g cm}^{-2} \ \text{d}^{-1})$ is proportional to the solute gradient:

$$J_{\text{dif}} = -\theta D_{\text{dis}} \frac{\partial c}{\partial z}$$

(13)

with $D_{\text{dis}} \ (\text{cm}^2 \ \text{d}^{-1})$ being the dispersion coefficient. Unless water is flowing very slowly the dispersion flux is usually much larger than the diffusion flux.

The total solute flux density $J \ (\text{g cm}^{-2} \ \text{d}^{-1})$ is therefore described by the sum:

$$J = J_{\text{dif}} + J_{\text{con}} + J_{\text{dis}} = q c - \theta (D_{\text{dif}} + D_{\text{dis}}) \frac{\partial c}{\partial z}$$

(14)

**Transport Equation**

By considering the conservation of mass in an elementary volume, we may derive the continuity equation for solute transport:

$$\frac{\partial X}{\partial t} = -\frac{\partial J}{\partial z} - S_s$$

(15)

where $X$ is the total solute concentration in the soil system (g cm$^{-3}$) and $S_s$ is the solute sink term, which accounts for decomposition and uptake by roots (g cm$^{-3} \ \text{d}^{-1}$). The solutes may be dissolved in soil water and/or may be adsorbed to organic matter or to clay minerals:

$$X = \theta c + \rho_b Q$$

(16)

with $\rho_b$ being the dry soil bulk density (g cm$^{-3}$) and $Q$ the amount adsorbed (g g$^{-1}$). The adsorption isotherm describes the amount of solutes adsorbed in equilibrium with the dissolved concentration $c$. In SWAP we assume instantaneous equilibrium between $c$ and $Q$ and use the non-linear Freundlich equation, which is a flexible function applicable to many organic and inorganic solutes. Freundlich adsorption can be written as:

$$Q = K_f c_{\text{ref}} \left( \frac{c}{c_{\text{ref}}} \right)^{N_f}$$

(17)

with $K_f$ being the Freundlich coefficient (cm$^3$ g$^{-1}$), $N_f$ the Freundlich exponent (-), and $c_{\text{ref}}$ a reference solute concentration (g cm$^{-3}$), which is used to make $N_f$ dimensionless. The solute sink term $S_s$ accounts for first order transformation and proportional root uptake:

$$S_s = \mu (\theta c + \rho_b Q) + K_f S_a c$$

(18)

where $\mu$ is the first order rate coefficient of transformation (d$^{-1}$), $K_f$ is the root uptake preference factor (-), and $S_a$ is the root water extraction rate (d$^{-1}$). The transformation rates of the dissolved and adsorbed solutes are assumed to be equal. $K_f$ accounts for positive or negative selection of solute ions relative to the amount of solutes present in soil water extracted by the roots.

The transformation rate coefficient is affected by soil temperature, water content and depth. Analogous to Boesten and Van der Linden (1991), SWAP calculates $\mu$ from:

$$\mu = f_T f_0 f_z \mu_{\text{ref}}$$

(19)

in which $f_T$ is a soil temperature factor (-), $f_0$ and $f_z$ are reduction factors (-) accounting
for the effect of soil water content and soil depth, and $\mu_{\text{ref}} \, (\text{d}^{-1})$ is $\mu$ at reference conditions (e.g. soil from the plough layer at 20 °C and at soil water pressure head $h = -100 \, \text{cm}$).

Combination of Eqs. 14, 15, 16 and 18 yields the transport equation applied in SWAP which is valid for dynamic, one-dimensional, convective-dispersive mass transport, including non-linear adsorption, linear decay and proportional root uptake in unsaturated/saturated soil (e.g. Boesten and Van der Linden, 1991):

$$\frac{\partial (\theta c + \rho_s Q)}{\partial t} = - \frac{\partial q_c}{\partial z} + \frac{\partial}{\partial z} \left( \theta \left( D_{\text{diff}} + D_{\text{adv}} \right) \frac{\partial c}{\partial z} \right) - \mu (\theta c + \rho_s Q) - K_s Sc \quad (20)$$

An explicit, central finite difference scheme is used to solve Eq. 20 (Dam van, et al., 1997). The solute transport processes incorporated in SWAP permit the simulation of ordinary salt and pesticide transport, including the effect of salinity on crop growth.

**SWAP INTERFACE**

SWAP can be used with or without graphical user interface. Researchers and more experienced SWAP users might prefer to work without the graphical user interface, as input and output files are accessible faster and ASCII output data can be imported in personal graphical packages. Also changes to the program code which affect model input or output, require less effort without the graphical user interface. Use of SWAP with the plain ASCII in- and output files is documented by Kroes et al., (1999).

The graphical user interface (Huysgen et al., 2000), written in Delphi, facilitates data input and analysis of simulation results. For instance at the input side, the format of weather data can be changed easily, soil hydraulic functions can be generated from soil texture, time dependent input data can be viewed to check consistency, and depending on earlier selected options, not relevant input data are hidden. At the output side, soil profile data on water content, solute concentration and temperatures can be compared graphically between dates or scenario’s, water and solute balances can be viewed graphically and the correlation between a large number of water, solute, heat and plant growth variables can be examined.

**CONCLUSIONS**

Current developments with multi-dimensional, physically based models and integrated hydrological frameworks, will further improve our analysis of water and solute movement in soils. Because of their flexibility, accessibility and speed however, the coming decade 1D-models like SWAP will keep to play an important role to explore new flow concepts, to analyse laboratory and field experiments, to select viable, water management options, to perform regional studies employing geographical information systems and to illustrate transport processes for education and extension.

**AVAILABILITY OF SWAP**

The program can be downloaded from the Internet. The SWAP2.0 package consists of the following elements: 1) SWAP source code; 2) SWAP executable; 3) Graphical User Interface; 4) Case study with basic exercises; 5) Data base with daily meteorological data (Wageningen, 1954-1993), soil physical data (Dutch national data base: Staring Series) and crop growth data of 10 Western European crops; 6) Presentations which introduce SWAP and describe its soil water flow features. This package can be downloaded without costs by co-workers and students of the Wageningen University- and Research centre (WUR). Users outside WUR should pay once 1000 DG for SWAP development and management.

The following procedure is followed. At the Internet site, the user registrates his name and address and downloads the package SWAP2.0. Next Alterra sends the bill. After payment, Alterra sends the manuals on theory, program use and the graphical user interface.

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interface. Registrated user's are free to download future SWAP versions.

**Literature Cited**


Figures

Fig. 1. Schematization of hydrological processes incorporated in SWAP.

Fig. 2. Schematization of the crop growth processes incorporated in WOFOST.
Fig. 3. Reduction coefficient for root water uptake, $\alpha_{rw}$, as function of soil water pressure head $h$ and potential transpiration rate $T_p$ (after Feddes et al., 1978).

Fig. 4. Reduction coefficient for root water uptake, $\alpha_{rs}$, as function of soil water electrical conductivity $EC$ (after Maas and Hoffman, 1977).
Fig. 5. Schematization of local drainage and regional bottom flux in SWAP.