# Soil Parameterization for Dynamic Simulation of Land Qualities

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### 1. Introduction

Water is usually the factor limiting crop production. Calculations of water-limited production potential are dependent on the complex land quality 'water availability during the growing season'.

Shortage of water affects the rate of assimilation by a factor CFWATER, which expresses the relative sufficiency of water availability: CFWATER is the ratio of the actual transpiration rate (dictated by water supply) and the maximum transpiration rate (conditioned by water demand). The sufficiency of water availability is calculated in a water balance, where the state variable is the actual volume fraction of soil moisture (SMPSI).

The model used is a comprehensive, deterministic crop production model, developed for dynamic simulation of land qualities and corresponding land use requirements, in rigidly defined production situations (Driessen and Konijn, 1992). Field experimentation was carried out at the experimental farm of the Institute for Natural Resources and Agrobiology of Seville (IRNAS) in Coria del Rio, Spain. Selected land-use systems with sunflower were monitored in 1993 and 1994.

### 2. Materials and Methods

The rooted surface soil is treated as one compartment; its upper boundary is the soil surface and its lower boundary is at an equivalent rooting depth that changes over the growing season. The sources of water in the water balance are precipitation, irrigation and capillary rise, evaporation, transpiration, surface runoff and deep percolation/drainage, act as sinks.

The rate of change of the volume fraction of moisture in the rooted surface compartment (RSM) depends on the fluxes of water (vapour) through its two boundaries and on water extraction by roots for transpiration.

Water fluxes through the lower boundary of the rooted surface compartment are composed of deep percolation (D) and capillary rise (CR). Both processes follow the general flow equation. The depth of the phreatic level (ZT), may be fixed e.g. in the case of forced drainage, or vary over the season. The change in depth of the phreatic level (DeltaZT) is made dependent on the rise of the ground water by a predominance of deep percolation or by its fall as a result of capillary rise.

The actual rate of transpiration (TR) is found by matching the maximum rate of water uptake by roots (MUR) and the theoretical maximum rate of transpiration (TRM). MUR is the result of the difference in water potential between the soil and the plant, and the respective root and plant resistances to the water flow. It represents the supply side. TRM, the

demand side, is calculated from the potential rate of evapotranspiration corrected for actual soil cover and the effects of air turbulence. If MUR  $\geq$  TRM then TR = TRM else TR = MUR.

Fluxes through the upper soil (UPFLUX) are the result of many processes. A mulch layer forms at soil surface if evaporation losses are not fully replenished. Actual evaporation is found by matching maximum vapour flux through the mulch layer (VAPFLUX) and the rate of upward water flow to the lower boundary of the mulch layer (WATSUPPLY) with the maximum rate of evaporation (EM). VAPFLUX is calculated from the vapour pressure gradient (between the mulch layer and the rooting zone) and diffusion coefficients. WATSUPPLY is calculated as vertical flow; EM is calculated by correcting the evaporation rate from a bare soil for shading by the crop canopy. The actual rate of evaporation, EA, is found by matching the supply side, given by WATSUPPLY or VAPFLUX (whichever has the smaller value), with the demand EM. The smaller value is retained as the actual rate of water vapour loss.

The gross rate of water supply to the upper boundary of the rooted soil compartment (GROSSUP) is equal to precipitation plus irrigation, diminished by the actual evaporation losses of water from the soil surface. This gross supply enters the mulch layer; any surplus constitutes the net rate of water supply to the underlying root zone (NETSUP).

Infiltration of surface supply into the soil is conditioned by the soil's infiltration capacity (IM), which is determined by matric forces and gravity forces. NETSUP is matched with the momentary infiltration capacity. Excess supply increases surface storage of water for future release to the rooting zone (DS); or is lost by surface runoff (SR). Runoff occurs only when the surface storage capacity (SSC) is exceeded. SSC represents the equivalent water layer that can be stored on top of the land and is a function of the slope and surface properties of the land.

The equivalent rooting depth (RD) varies from a initial value at the beginning of the growing season till a maximum value reached when root growth ceases (RDSroot). Between these two limits, the increase of rooting depth over time is assumed linear (DeltaRD).

The initial values of all state variables at the beginning of the crop cycle are defined. For each time interval (Dt) they are then adjusted with the results of the water budget calculations.

Essential (pedo)transfer functions in this water balance model are those defining:

•	Moisture retention by the soil SMPSI = SMO * PSI <sup>-GAM*In(PSI)</sup>	(1)
•	Hydraulic conductivity of the soil KPSI = KO * EXP(-ALFA * PSI) at low suction KPSI = AK * PSI <sup>-n</sup> at high suction where the boundary between low and high suction is given by PSImax.	(2.a) (2.b)
•	Vertical flow of water in the soil Flow = KPSI * (PSI gradient/ Distance - 1)	(3)
•	Infiltration of water in the soil IM = SPSI * Dt-0.5 + Ktr with SPSI = SO * (1 - SMPSI / SMO)	(4.a) (4.b)

where:	
PSI	i matric suction of rooted soil (cm).
SMO	is total pore fraction (cm3.cm-3).
GAM	is texture-specific constant (cm-2).
SMPSI	is volume fraction of moisture in soil with suction PSI (cm3.cm-3).
KPSI	is hydraulic conductivity of soil with matric suction PSI (cm.d-1).
KO	is saturated hydraulic conductivity (cm.d-1).
ALFA	is texture-specific geometry constant (cm-1).
AK	is texture-specific empirical constant (cm-2.4.d-1).
Ν	is empirical constant, in practice n = 1.4 for all soil materials.
PSImax	is texture-specific suction boundary (cm).
SO	is reference sorptivity (cm.d-0.5).
SPSI	is actual sorptivity (cm.d-0.5).
Ktr	is hydraulic permeability of transmission zone (cm.d-1).

The main goal of the water balance module is to quantify the soil moisture content over the crop season and derive the sufficiency of water availability for crop production.

The soils of the experimental farm at Coria del Rio are Calcaric Cambisols, as defined by the FAO-Unesco classification system (FAO-Unesco, 1988). Cambisols are mineral soils of limited genetic age. They show beginning horizon differentiation through changes in colour, and/or structure, and are formed from medium to fine-textured materials, mostly in colluvial, alluvial or eolian landscapes (Driessen and Dudal, 1989). Calcaric Cambisols show strong effervescence with 10 % hydrochloric acid. The soil temperature regime is thermic and the moisture regime is xeric.

The landform is an alluvial plain with flat topography. The land element is a terrace in the higher part of the alluvial plain, adjacent to undulating lower hills.

The soil parent material consists of alluvial and colluvial deposits, and is derived from limestone. The effective soil depth is 'very deep'; the soil texture is loamy (25 % clay, 31 % silt and 44 % sand), with a bulk density of 1.34 g.cm<sup>-3</sup> and a porosity of 0.50 cm<sup>3</sup>.cm<sup>-3</sup>. The soils may show vertic properties, albeit that cracks are normally too shallow for the soils to classify as vertic. The soils shrink as witnessed by the ratio of bulk densities of wet over dry samples: 0.89.

The soil surface is free of rock outcrops but may contain very few coarse fragments. There is no evidence of erosion. The soil-water regime is characterized by rapid internal drainage; the soils are rarely saturated with water and lack external drainage. The soils have a moderate hydraulic conductivity and a very deep ground water table.

Common chemical soil properties are a field pH of 7.5, an ECe value of 0.25 mS.cm-1, a carbonate content of 29 %, a C/N ratio of 10 and average NPK values around 0.07 %, 28 mg.kg-1 and 293 mg.kg-1 respectively. The organic matter content is around 1 %.

The land is planted with sunflower, cotton, wheat and sugarbeet. The soils are modified by tillage, irrigation, application of fertilizers and chemicals, and by mechanized cultivation and harvest practices.

Field measurements and laboratory soil analyses include:

- Double ring infiltration measurements.
- Hot-air method for measuring hydraulic conductivity at high soil suction.
- pF measurements.

- Bulk density measurements.
- Soil profile descriptions.
- Soil texture determinations.
- Gravimetric determinations of soil water content.
- Tensiometer readings.
- Multi-step outflow' determinations of hydraulic conductivity at low soil suction.

Parameterization of Coria del Rio soil produced the soil data shown in Table 1.

Moisture Retention	SM0 (cm3.cm-3) GAM (cm-2)	0.50 0.018
Hydraulic	KO (cm.d-1) ALFA (cm-1) AK (cm-2.4.d-1) PSImax (cm)	24 0.038 36 305
Infiltration	SO (cm.d-0.5) Ktr (cm.d-1)	11 0 5

Table 1.Soil Parameters

# 3. Results and discussion

The results of program runs for water-limited production potential scenarios were often quite different from measured field data. Attempts to correct this through adjustment of soil parameter values proved futile. The two figures below show selected state variables values over the crop season, where SMPSI is soil moisture content (-), CFWATER is water sufficiency (-), TR is actual rate of transpiration (cm.d-1) and MUR is maximum rate of water uptake by roots (cm.d-1). Note the sharp transitions in MUR and CFWATER values.







The high and low hydraulic conductivities in figures 1 and 2 are defined by the following set of parameters: in Fig. 1, AK=36 cm-2.4.d-1, n=1.4 and PSImax=181 cm; in Fig. 2, AK=36 cm-2.4.d-1, n=2.1 and PSImax=305 cm. Values of PSImax mark the transition from 'low suction' (eqn. 2.a) to 'high suction' (eqn. 2.b). Changes in the low suction equation are not

effective at soil suction values (far) beyond the PSImax value. This suggests that one or more parameter values must be changed. In this case the value of n was varied between 1.4 (recommended for all soil materials) and 2.1 (curve fitting).

In Fig. 1, CFWATER drops almost instantaneously from one (stress-free) to zero in response to a sharp drop in maximum uptake rate (MUR). In Fig. 2 transpiration is halted by soil saturation.

The actual rate of transpiration (TR) is found by matching water supply to the roots (MUR) with demand (TRM). The supply side represents the water available for transpiration: it depends on crop characteristics, crop development, and soil moisture content and soil hydraulics. The water required for maximum transpiration represents the demand side: it depends on environmental conditions and on crop characteristics and development. In Fig. 1, soil suction reached the PSIIeaf value and consequently the MUR value dropped to nil. In Fig. 2, the fluxes are so slow that water entering the system (in this case 9.2 cm of precipitation) increased the soil moisture content sharply until saturation.

To explain these two extremes, the soil data was compared with default soil data suggested for main textural classes (Driessen and Konijn, 1992).

Texture class	Coarse sands	Loamy sands	Sandy Loams	Loams	Clays	
SM0	0.4	0.45	0.5	0.47	0.5	
GAM	0.1	0.03	0.02	0.015	0.007	
K0	650	150	60	20	3	
ALFA	0.15	0.07	0.05	0.04	0.03	
PSImax	100	130	155	170	260	
AK	0.1	13	30	30	3	
<b>S</b> 0	50	20	17	17	5	
Ktr	430	100	40	14	2	

# Table 2. Indicative values for soil constants for reference soil texture classes

Using these constants and the equations for hydraulic conductivity (eqn. 2.a and 2.b) and soil moisture content (eqn. 1), the next two figures are constructed.









where the texture class cSa is coarse sand, LoSa is loamy sand, Sa is sand, Lo is loam, Cl is clay and CdR is the soil at Coria del Rio.

These two figures show that Coria del Rio soil behaves according to its textural class, both in terms of soil moisture content and hydraulic conductivity. Adjustment of soil parameters values and use of alternative soil conductivity equations produced the next figures: Fig. 5 shows LOG(KPSI) as a function of LOG(PSI) and Fig. 6 shows KPSI as a function of SMPSI.



# Figure 5.KPSI-PSI curves.Figure 6.KPSI-SMPSI curves.

Curves A, B and C are KPSI functions as in equations 2.a and 2.b; curve A with AK= 36 and n=1.4; curve B with AK=36 and n=2.1; curve C with AK=3 and n=1.4. Curve D is a KPSI function of the type of equation 5, with ALFA=0.19.

The explanation for the sharp changes in water balance variables can be seen in graphs 5 and 6. The problem is greatest in the pF range between 2 and 3. In the formal curve (A) the drop in KPSI is very steep. Attempts to smoothen the curve by means of 2 step equations bring no relief. Data obtained with the hot air method suggest a linear relationship beyond pF=3.2. Recall that KSPI values were obtained with measurements at PSI 50, 150, 500 and 1000 cm (pF 3) and extrapolated from thereon to higher PSI-values, i.e. to PSI values as occur in the cropping season. The differences between the curves A, B and C in Fig. 5 are evident despite the use of log scales, but such differences do not show up in Fig. 6.

There is evidently considerable variation in soil parameter values; soil sampling and sample treatment may explain part of the difference. Table 3. (Driessen, 1995) list generic values for construction of the hydraulic conductivity function (from literature).

Ranges and absolute values assigned to each texture class vary widely between authors. One source of difference may be in the determination of texture: "total clay contents" determined in the laboratory may differ significantly from field estimates of "natural clay". Less but broader texture classes would be adequate.

# Table 3.Generic values for the saturated hydraulic conductivity (K(sat) in cm.d-1)<br/>and for geometry coefficient ALFA (cm-1) as suggested by Rijtema (1969),<br/>Rawls et al. (1982), Carsel & Parrish (1988) and Wösten (1987).

Texture class	Rijtema (1969)		Rawls et al. (1982)		Carsel & Parrish(1688)		Wösten (1987)	
	K(sat)	ALFA	K(sat)	ALFA	K(sat)	ALFA	K(sat)	ALFA
Sand	1120	0.2440	504.0	0.138	712.8	0.145	223.0	0.0524
Loamy sand	26.5	0.0398	146.6	0.115	350.2	0.124	63.90	0.0182
Sandy loam	12	0.0248	62.16	0.068	106.1	0.075	53.10	0.0216
(Loess) loam	14.5	0.0490	16.32	0.090	24.96	0.036	25.60	0.0231
Silty loam	6.5	0.0200	31.68	0.048	10.80	0.020	24.00	0.0280
Sandy clayloam	23.5	0.0353	10.32	0.036	31.44	0.059	n.d.	n.d.
Clayloam	0.98	0.0248	5.52	0.039	6.24	0.019	n.d.	n.d.
Silty clayloam	1.5	0.0237	3.60	0.031	1.68	0.010	n.d	n.d
Sandy clay	3.5	0.0274	2.88	0.034	2.88	0.027	n.d	n.d
Silt clay	1.3	0.0480	2.16	0.029	0.48	0.005	n.d.	n.d.
Clay	0.22	0.0380	1.44	0.027	4.80	0.008	n.d.	n.d.

n.d. is not determined.

Considering the uncertainties associated with measured KPSI-data, a mathematical function for the description of KPSI is proposed that has the same structure as the moisture retention equation (eqn. 1):

KPSI = K0 \* PSI - ALFA \* In(PSI)where ALFA = 0.19 cm-2.

(5)

This equation produced the D curves in figures 5 and 6.

Soil parameters influence crop performance, especially where water availability to the root system is periodically marginal, but relevant soil parameters are difficult to quantify. Measured water retention curves are desorption curves that cannot be introduced in the calculations straightaway because in a field situation desorption and resorption alternate. Resorption curves may differ considerably from desorption patterns. The use of a theoretical function based on total pore fraction and a texture-specific pore geometry factor (optimized to fit measured values) avoids systematic over-estimation of water availability but can only be of a generic nature.

Another matter of concern is the dry bulk density value that is used to convert gravimetric water content to volumetric water content and to calculate total soil porosity: it is considered constant. However, bulk density values vary as a consequence of soil tillage and soil compaction. The accuracy suggested by tabulated total pore fractions and texture-specific pore geometry factors in the table of generic values for the soil moisture curve is therefore misleading; calculation results demonstrate that these soil parameters could well be aggregated to less but broader texture classes.

Water stored in the rooted soil compartment must flow to the roots before water lost in transpiration can be replenished. The resistance to flow is expressed by its reciprocal value, the (un)saturated hydraulic conductivity of the soil at the momentary soil moisture potential. The KPSI-PSI relation is particularly difficult to establish. Measurements are best done in situ but there are no reliable methods known that can handle soil suctions beyond 1000 hPa. In the land-use systems studied, drought is the problem (not waterlogging) and soil moisture potentials may exceed 15000 hPa. The only method that claims to deal with

such high suctions is the 'hot air method' but its operational value is generally considered to be low, inter alia because KPSI values are measured on a dislocated soil core of small volume that is hardly representative of an entire soil pedon, let alone of a field. Published KPSI-PSI relations extrapolate measured low-suction KPSI-values to the entire relevant KPSI range of 0 -> 15000 hPa, e.g. by extending a low suction KPSI-PSI relation (PSI <= 300 hPa) with a theoretical high suction function. The artificial nature of such broken curves and the (too) low flow rates suggested by them at PSI-values over a few thousand hPa makes it attractive to use an alternate notation that starts from the saturated hydraulic conductivity (K0) with a sigmoid KPSI-PSI pattern on the basis of a texture-specific pore geometry factor.

The main goal of the water budget calculations is to quantify the soil moisture content over the crop season as an indicator of the sufficiency of water for crop production. The effect of different hydraulic conductivity parameters can be evaluated by matching the generated soil moisture content with field measurements. Most of the variations found seemed caused by ALFA, a factor that expresses the effect of pore geometry on the KPSI-PSI relation. A higher ALFA value causes a lower KPSI and calculated water stress occurs later in the season.

### 4. Acknowledgements

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