## University of São Paulo "Luiz de Queiroz" College of Agriculture

Stochastic assessment of soil water balance components: development a	nd
application in a hardsetting soil scenario	

### **Arthur Klebson Belarmino dos Santos**

Thesis presented to obtain the degree of Doctor in Science. Area: Soil Science and Plant Nutrition

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### Arthur Klebson Belarmino dos Santos Agronomist

## Stochastic assessment of soil water balance components: development and application in a hardsetting soil scenario

versão revisada de acordo com a Resolução CoPGr 6018 de 2011

Advisor:

Prof. Dr. QUIRIJN DE JONG VAN LIER

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 Amostragem de solo 2. Método estocástico 3. Retenção de água no solo 4. Condutividade hidráulica 5. Componentes do balanço hídrico I. Título To my mother Quitéria Belarmino To my father Amaro Antônio To my sister Marianne Belarmino

### I DEDICATE!

"Before you judge my life or my character, put on my shoes and walk the path I've walked. Long live my sorrows, my doubts and my fears, my pain and my laughter. Walk through the years I've walked, stumble where I've stumbled, and pick yourself up - just like I did. And then, only then you can judge me. Each person has their own story. Don't compare your life to that of others. You don't know what the path they had to walk in life was like."

Unknown

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#### **RESUMO**

## Avaliação estocástica dos componentes do balanço hídrico do solo: desenvolvimento e aplicação em um cenário de solo coeso

A modelagem hidrológica é uma ferramenta essencial para a compreensão dos processos que ocorrem na zona vadosa do solo. Esses processos são dependentes de parâmetros de retenção de água no solo e da condutividade hidráulica, que normalmente são determinados em réplicas de amostras de solo não deformadas. No entanto, esse método não é eficaz quando se objetiva representar grandes áreas, pois geralmente é utilizada a média de todas as repetições. Com base nisso, apresenta-se um método para mesclar os parâmetros hidráulicos do solo de todas as repetições em um único conjunto de dados com suas estatísticas associadas (erros padrão e matriz de correlação). Para tanto, utilizaram-se parâmetros de van Genuchten-Mualem (VGM) de três repetições de um solo coeso de Cerrado da região leste do estado do Maranhão, Brasil, obtidos por meio de modelagem inversa de experimentos de evaporação em laboratório. A eficácia e a representatividade da metodologia proposta foram avaliadas observando-se a distribuição de frequências dos parâmetros, comparando-se as propriedades das amostras individuais e as mescladas (parâmetros VGM, características de retenção e condutividade hidráulica e componentes do balanço hídrico) previstas estocasticamente por um modelo hidrológico. Com o método estabelecido, ele foi utilizado em uma série histórica de 31 anos com resultados das três amostras coletadas em três profundidades (0-15, 15-30 e 30-45 cm) do solo. O método estocástico permitiu obter a variabilidade das repetições mescladas para os componentes do balanço hídrico. Aplicando a técnica ao período de 31 anos, alguns conjuntos de parâmetros de VGM gerados, bem como o acúmulo e distribuição de chuvas durante o ciclo das culturas se mostraram fatores determinantes para a dispersão dos resultados dos componentes simulados do balanço hídrico. Com exceção dos dados de transpiração, os demais componentes do balanço hídrico (drenagem profunda, evaporação e runoff) apresentaram boa correlação com a precipitação acumulada. Uma redução significativa na dispersão da taxa de transpiração foi notada em anos com alta precipitação. Em geral, o uso dos valores médios dos parâmetros das propriedades hidráulicas para prever deterministicamente os componentes do balanço hídrico pode produzir valores que são substancialmente diferentes dos valores medianos das realizações estocásticas. Isso sugere que esses valores podem gerar resultados não representativos na modelagem hidrológica, demonstrando o papel importante da modelagem estocástica.

Palavras-chave: Amostragem de solo, Método estocástico, Retenção de água no solo, Condutividade hidráulica, Componentes do balanço hídrico

#### **ABSTRACT**

## Stochastic assessment of soil water balance components: development and application in a hardsetting soil scenario

Hydrological modelling is an essential tool for understanding the processes that occur in the soil vadose zone. These processes are dependent on soil water retention parameters and hydraulic conductivity, which are normally determined using replicas of undisturbed soil samples. However, this method is not effective when trying to represent large areas, since an average of all replicas is usually performed. Based on this, we present a method to merge the hydraulic soil parameters of all replicas into a final set of data, with their associated statistics (standard errors and correlation matrix). To do so, we used VGM parameters obtained at sample scale in three replicas from a Brazilian savanna hardsetting soil from the eastern part of Maranhão state, Brazil through inverse modelling of laboratory evaporation experiments. The effectiveness and representativeness of the proposed methodology were evaluated by observing the frequency distribution of the output parameters, and comparing individual and merged sample properties (VGM parameters, retention, and hydraulic conductivity characteristics together with soil water balance components) stochastically predicted by a hydrological model. With the established method, a 31-year historical data set was analysed for three samples collected at three depths (0-15, 15-30, and 30-45 cm) in the hardsetting soil. The stochastic method allowed obtaining the variability of the combined replicas for the water balance components. Applying the technique to the 31 years, some generated VGM parameter sets, as well as the rainfall accumulation and distribution during the crop cycles, showed to be the determining factors for the dispersion of the simulated water balance components. Except for transpiration data, the other water balance components (bottom flux, evaporation, and runoff) showed a good correlation with the accumulated precipitation. A significant reduction in the dispersion of the transpiration rate was observed in high precipitation years. In general, using the mean hydraulic property parameter values to deterministically predict water balance components may yield values that are substantially different from the median values of stochastic realizations. This suggests that these values may generate unrepresentative results in hydrological modelling, showing the important role of stochastic analysis.

Keywords: Soil sampling, Stochastic method, Soil water retention, Hydraulic conductivity, Water balance components

#### 1. INTRODUCTION

The evaluation of soil water dynamics and water balance components in the vadose zone is strongly determined by the water retention and hydraulic conductivity functions controlling any soil water flow process (Angaleeswari & Ravikumar, 2019; Sheikhbaglou et al., 2021). In this context, the use of process-based hydrological models, simulating soil water flow using a numerical solution of the Richards equation, stands out as an important tool for water balance prediction and crop productivity components. Among these models, some of the most widespread are Hydrus (Šimůnek et al., 2016), DSSAT-Hydrus-1D (Shelia et al., 2018), and SWAP (Kroes et al., 2017). In addition, to predict water balance and crop productivity components, these models also predict processes such as solute transport (Chen et al., 2019), root water uptake (Leiet al., 2021), the fate of soil pollutants (Shelia et al., 2018) and groundwater recharge (Ma et al., 2015).

Normally, the application of these models to access K- $\theta$ -h is performed in a deterministic approach, using the mean parameters of the hydraulic functions. Whichever model or method is chosen, when performing a deterministic simulation, the generation of uncertainties, inherent to the process, is not possible (de Jong van Lier et al., 2019; Pinheiro & de Jong van Lier, 2021). Using a stochastic technique, the confidence interval and correlations between parameters of these functions can be included in the simulations, allowing the prediction of uncertainties associated with the predicted water balance components.

We present a novel method for merging soil hydraulic properties and associated uncertainties of several soil samples into a single set of parameters that can be applied in stochastic simulations. The method was applied using soil hydraulic parameters obtained from the inverse modelling of evaporation experiments in samples of a hardsetting soil from the eastern region of the state of Maranhão, Brazil, cultivated with soybean-millet rotation. To assess the effectiveness and representativeness of the proposed methodology, the frequency distribution of different outputs was analysed, including the van Genuchten-Mualem parameters, retention and conductivity characteristics, and water balance components stochastically predicted by the SWAP 1D hydrological model. After evaluating the efficiency of the stochastic method, it was considered successful and applied to a 31-year climate series to predict the water balance components bottom flux, evaporation, transpiration, and runoff. For this, a 31-year history series was used (1990 to 2020) in a hardsetting soil.

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# 2. STOCHASTIC MERGING OF SOIL HYDRAULIC PROPERTIES FOR VADOSE ZONE HYDROLOGICAL MODELLING

Arthur Klebson Belarmino dos Santos<sup>1</sup>, Majken Caroline Looms<sup>2</sup>, Quirijn de Jong van Lier<sup>3</sup>

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#### **Abstract**

Soil hydraulic properties (SHP) are commonly determined in soil samples with replicas. Whether these replicas are taken at a same location to represent a specific point or at several locations to represent a larger area, results should be merged into a final dataset to be used in modelling. For this dataset to be representative, standard errors and correlation matrix must be considered in the merging process. We present a method to perform this merging and give an example using stochastic realizations of van Genuchten-Mualem (VGM) parameters generated by Cholesky decomposition to merge the SHP and associated statistics into a merged parameter set. To do so, we used VGM parameters obtained at sample-scale in three replicas from a Brazilian savanna soil through inverse modelling of laboratory evaporation experiments. The effectiveness and representativeness of the proposed methodology were evaluated by observing the frequency distribution of different levels of output, comparing individual and merged sample properties. The outputs include VGM parameters, retention and conductivity characteristics, and water balance components stochastically predicted by a hydrological model. The performed stochastic merging correctly represented the variability of the combined replicas, especially with respect to hydrological model outputs of soil water balance components. Using the mean hydraulic property parameter values to deterministically predict water balance components may yield values that are substantially different from the mean values of stochastic realizations. This suggests that the deterministic prediction using mean parameter values in vadose zone hydrological modelling may result in unrepresentative outputs.

Keywords: Soil water retention; Hydraulic conductivity; Soil water balance; Soil sampling.

#### 2.1. Introduction

Hydrological modelling is an important tool for the prediction of soil water balance components and decision-making regarding water management of agricultural and natural systems. Process-based hydrological models require the input of soil hydraulic parameters describing water retention and hydraulic conductivity.

<sup>&</sup>lt;sup>1</sup> Soil Science Department, "Luiz de Queiroz" College of Agriculture, University of São Paulo, Piracicaba, SP 13418-900, Brazil

<sup>&</sup>lt;sup>2</sup>Department of Geosciences and Natural Resource Management, University of Copenhagen, Øster Voldgade 10, 1350 Copenhagen, Denmark

<sup>&</sup>lt;sup>3</sup>Tropical Ecosystem Division, Center for Nuclear Energy in Agriculture (CENA), University of São Paulo, Piracicaba, SP 13416-903, Brazil

There are several available techniques for obtaining soil hydraulic properties (SHP). Laboratory equilibrium measurement methods include one-step outflow experiments (Kool et al., 1985; Watson, 1967) and multi-step outflow experiments, in which an initially saturated sample is equilibrated at a predefined pressure using a porous plate or other medium. Another widely used technique is the transient observation of the water tension in a sample during evaporation experiments, allowing the determination of SHP by inverse modelling (Schindler & Müller, 2006; Wendroth et al., 1993; Wind, 1969). Alternatively, soil moisture data series obtained during forced or natural infiltration in the field can also be used in inverse modelling approaches to obtain SHP (Filipović et al., 2018). Finally, pedotransfer functions can be used to estimate SHP from available information about, e.g., particle size distribution, organic matter content, and bulk density (Schaap et al., 2001; Twarakavi et al., 2009; Singh et al., 2021).

Whichever method is used, uncertainty will be associated to the resulting SHP parameters. In laboratory methods applied to soil samples, the resulting information contains uncertainty due to inherent soil variability within the sample, measurement precision, and/or non-uniqueness in inverse estimation. This uncertainty can be expressed in terms of a standard error. When dealing with more than one descriptive parameter, as in the case of soil hydraulic functions, correlations between the parameters are quantified in a correlation matrix. Whichever measurement method is used, resulting hydraulic parameters represent a small sample and refer to a specific field location. To increase the representability for a larger area like a field or soil mapping unit, samples at more locations (replicas) are commonly taken. Especially when evaluating a complex system such as a cultivated soil, higher variability may be expected for some soil properties and more or larger samples would be needed to better describe the soil or the soil layer (Koestel et al., 2020; Pachepsky & Hill, 2017). Each replica yields a set of deterministic values or a set of stochastic values for the hydraulic parameters with respective means, standard errors, and correlation matrix.

There are some approaches for merging sample information into one set of SHP to represent the joint set of samples, such as from three-dimensional geostatistical models (Fleckenstein & Fogg, 2008), Bayesian neural networks (Jana et al., 2012), and critical path analysis (Ghanbarian et al., 2017). However, these methods do not preserve the information about standard errors and correlation matrix present in the individual sample measurements, needed to allow the generation of stochastic realizations for a Monte Carlo simulation approach. Opposed to the results of a deterministic study represented by one simple model output using the mean parameter values, a Monte Carlo (stochastic) modelling yields a

distribution of outputs with mean and standard deviations or uncertainties of the model outputs. Not including the parameter correlation has been shown to increase the uncertainty of stochastic modelling output (Pinheiro & de Jong van Lier, 2021).

Our objective was to present a method which enables the merging of the SHP and associated statistics of several samples into a single parameter set that can be used for stochastic simulations representing an entire set of samples. We present an example of an application with data obtained from the inverse modelling of laboratory evaporation experiments performed in samples of a tropical soil from Brazil. To evaluate the effectiveness and representativeness of the proposed methodology, the frequency distribution of different levels of output using individual and merged sample properties will be compared. The outputs include van Genuchten-Mualem parameters, retention and conductivity characteristics, and water balance components stochastically predicted by a hydrological model.

#### 2.2. Material and Methods

#### 2.2.1. Soil hydraulic properties

In this study, the soil hydraulic properties are described by the van Genuchten-Mualem (VGM) analytical K- $\theta$ -h functions (Mualem, 1976; van Genuchten, 1980):

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

$$K = K_{sat} \Theta^{l} \left[ 1 - \left( 1 - \Theta^{\frac{n}{n-1}} \right)^{1 - \frac{1}{n}} \right]^{2}$$
 (2)

where  $\Theta$  is the effective saturation,  $\theta$  (cm<sup>3</sup> cm<sup>-3</sup>) is the volumetric water content, h (cm) is the pressure head, and K (cm d<sup>-1</sup>) is the unsaturated hydraulic conductivity. In these equations, six parameters define the soil hydraulic properties and will be referred to as the van Genuchten-Mualem (VGM) parameters:  $\theta_r$  (residual water content, cm<sup>3</sup> cm<sup>-3</sup>),  $\theta_s$  (saturated water content, cm<sup>3</sup> cm<sup>-3</sup>),  $K_s$  (saturated hydraulic conductivity, cm d<sup>-1</sup>), and shape parameters  $\alpha$  (cm<sup>-1</sup>), n (-), and l (-).

#### 2.2.2. Sampling information

Undisturbed soil samples (volume 95.8 cm<sup>3</sup>; height 7 cm; internal diameter 7.4 cm) were collected in the surface layer (0-15 cm depth) of a native area of the Brazilian savanna in Maranhão State, Brazil (3°16'59"S 43°28'52"W). The soil is classified as a Haplic Acrisol (IUSS Working Group WRB-FAO, 2015) with loamy sand texture (0.819 kg kg<sup>-1</sup> sand, 0.055 kg kg<sup>-1</sup> silt, and 0.126 kg kg<sup>-1</sup> clay). The sampling location has a Koeppen Aw climate (Tropical savanna climate with dry-winter characteristics) with an annual rainfall of 1670 mm and a mean temperature of 27 °C.

#### 2.2.3. Obtaining a set of VGM parameters

#### **Evaporation experiments**

Soil samples were saturated by capillary rise from bottom to top for 48 h. Subsequently, repeated measurements of gamma-ray attenuation and sample weight were made every 24 h until negligible weight change (< 1 g d<sup>-1</sup> equivalent to < 0.01 m<sup>3</sup> m<sup>-3</sup> d<sup>-1</sup>). The samples were weighed, and the water content was measured by gamma-ray attenuation using a 3 mm diameter collimated <sup>137</sup>Cs beam. Readings were made twice at each of five vertical positions in the sample: 1.0, 1.5, 2.0, 3.5, and 5.0 cm below the sample surface. The counting time was 20 s for each reading. Subsequently, the sample was kept in the laboratory to evaporate from the upper surface, with a controlled temperature between 18 and 21 °C. At the end of the experiment, the final water content was determined by oven drying at 105 °C for 24 h and a final gamma reading in the oven-dry sample was performed. The evaporation rate between subsequent series of measurements was determined by weight difference. Attenuation readings were transformed to water content using the Beer-Lambert attenuation law (Wang et al., 1975) together with the attenuation coefficient of pure water and of the soil particles, determined from the final oven-dry reading.

#### **Inverse problem optimization**

The inverse modelling option of Hydrus-1D (Šimůnek et al., 2016a) was used to obtain the hydraulic parameters and associated statistics for each sample. Hydrus-1D simulates one-dimensional variable-saturated water flow in porous media by numerically solving the Richards equation. The Marquardt-Levenberg algorithm is used for inverse problem optimization. The boundary conditions were set to reflect the measured evaporation flux at the upper boundary and a zero flux at the lower boundary.

Measured water contents over depth and time together with measured evaporation rates were used to compose the objective function to be minimized by Hydrus-1D. As a result, Hydrus produces an estimate of the parameters from Eqs. [1] and [2] as well as respective standard errors and correlation matrix. To reduce the uncertainties of the parameter estimates, fixed values of  $\theta_r = 0$  and  $K_s = 60$  cm d<sup>-1</sup> were assumed.  $\theta_r$  was fixed at this value because, in all simulations, its value converged to zero, and the used value of  $K_s$  corresponds to measurements performed in soils from the region. The remaining four parameters ( $\theta_s$ ,  $\alpha$ , n, and l) were obtained by the inverse modelling.

#### 2.2.4. Merging statistical properties of hydraulic parameters from replicas

The inverse modelling procedure resulted in mean values and standard errors for each parameter, together with the correlation matrix. To merge the statistical properties of several replicas into one set of information (merged means, standard errors, and correlation matrix) while preserving the properties of the individual replicas, stochastic realizations of the parameter set for each sample were generated. These sets of realizations of all the replicas were joined together and the properties of the resulting merged dataset were calculated.

To generate the stochastic realizations for each sample, Cholesky decomposition was used (Davis, 1987; Minasny & McBratney, 2018; Pinheiro & de Jong van Lier, 2021). Considering the parameters from Eqs. [1] and [2] to be characterized by their means ( $\mu_i$ ), standard errors ( $\sigma_i$ ) and a correlation matrix, the covariance matrix ( $\Sigma$ ) is determined.  $\Sigma$  is then decomposed into a lower triangular matrix (L) so that the product of the lower triangular matrix (Cholesky decomposition factor) L and its transpose  $L^T$  gives back  $\Sigma$ :

$$\Sigma = LL^{T} \tag{3}$$

Subsequently, a vector Z of independent random normally distributed numbers with mean 0 and variance 1, of length equal to the dimensions of L is generated. This is done by generating a corresponding vector of linear random values R between 0 and 1, and calculating the value yielding R as the cumulative probability for a normal distribution with mean 0 and standard error 1. Optionally, a tail fraction  $\tau$  may be excluded at both extremities of the distribution curve to avoid outlying parameter values, in which case the random vector R will be generated between  $\tau$  and  $1-\tau$ . We used  $\tau=0.03$  in our analysis. Based on the vector Z, a number k of stochastic realizations of parameters are simultaneously computed by multiplying by L and adding the mean value for each hydraulic parameter:

$$x_i = LZ + \mu_i \tag{4}$$

where  $x_i$  represents the random variable vector for parameter i and  $\mu_i$  is the mean value of the respective parameter.

Due to the randomness of the procedure, the number of stochastic realizations k should be sufficiently large to guarantee the similarity (or stability) of the statistical properties (standard errors and correlation matrix) of the k realizations, which should be similar to the input data. The stability was tested with five values of k ( $k = 10^2$ ,  $10^3$ ,  $10^4$ ,  $10^5$ ,  $10^6$ ) by using the procedure to generate 10 sets (repetitions) of random realizations for each k and verifying the root mean square error (RMSE) of these when compared to the original sample values.

#### 2.2.5. Verification of the merged statistical properties

To verify the effectiveness of the process of merging the sample property values, evaluations were performed at three levels.

A first-level verification consisted of the comparison of the original three samples data and the merged data set regarding the frequency distribution of values of the four predicted parameters. A second-level comparison was performed by comparing the frequency distribution of water content and hydraulic conductivity at selected pressure heads calculated using stochastic parameter realizations from the individual samples and the merged parameter set. A third-level comparison was based on the comparison of the frequency distribution of selected outputs of the hydrological model SWAP (Kroes et al., 2017) using stochastic realizations from individual and merged sample properties. SWAP performs a dynamic Richards equation-based modelling of vertical soil water flow based on soil hydraulic properties, with specific options to include crop characteristics, meeting well the requirements of this study.

The SWAP 1D hydrological model employs a discretized form of the Richards equation (van Dam & Feddes, 2000) including a root water extraction sink term, according to

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + 1 \right) \right] - S(h)$$
 (5)

where C(h) is the differential water capacity  $(\partial \theta/\partial h, [\text{cm}^{-1}])$ , t is time [d], z is the vertical coordinate taken positive upwards [cm], h is the pressure head [cm], K(h) is the hydraulic conductivity [cm d<sup>-1</sup>] and S(h) represents water uptake by plant roots [d<sup>-1</sup>]. The numerical

solution of Eq. (5) requires parameterizing the unsaturated soil hydraulic properties (K- $\theta$ -h), here described by the analytical functions from the van Genuchten-Mualem model [Eqs. (1) and (2)].

SWAP model outputs include cumulative soil water balance components bottom flux, transpiration, evaporation, and runoff. These were simulated for a rainfed soybean scenario using a crop cycle of 120 days with a maximum rooting depth of 0.4 m. Temperature sum from emergence to anthesis and from anthesis to maturity, both used to calculate the development stage, were taken as 990 and 840  $^{\circ}$ C d respectively with a basal temperature of 10.0  $^{\circ}$ C.

A soil profile depth of 1.5 m was used in the simulations. The bottom boundary condition was set to free drainage (gravitational flow) and the upper boundary condition was described in terms of potential evapotranspiration ( $ET_p$ ) and precipitation. The SWAP model partitions  $ET_p$  further into potential transpiration ( $T_p$ ) and potential evaporation ( $T_p$ ) according to the leaf area index.

When integrated over depth, the root water uptake term S(h) in Eq. (4) corresponds to the actual transpiration ( $T_a$  [cm d<sup>-1</sup>]) which is calculated according to a modified version of the transpiration reduction function proposed by Feddes et al., 1978.  $T_a$  [cm d<sup>-1</sup>] is calculated by multiplying the potential transpiration  $T_p$  [cm d<sup>-1</sup>] by an empirical factor  $\varphi_z$ , evaluated for each soil layer (z) and weighted by the layer thickness  $w_z$  [L] and the relative root length density in the respective layer ( $R_z$ ):

$$T_a = T_p \frac{\sum_{z=1}^{z} \left[ \varphi_z w_z R_z \right]}{\sum_{z=1}^{z} w_z R_z}$$
 (6)

The empirical reduction factor  $\varphi_z$  ( $0 \le \varphi_z \le 1$ ) is defined by four threshold pressure head values ( $h_4 < h_3 < h_2 < h_1 \le 0$ ). Below wilting point ( $h < h_4$ ) and in the anoxic phase ( $h > h_1$ ),  $\varphi_z = 0$ ; in the falling rate phase ( $h_4 < h < h_3$ ),  $\varphi_z = (h - h_4)/(h_3 - h_4)$ ; in the constant (optimum) rate, delimited by  $h_3$  and  $h_2$ ,  $\varphi_z = 1$ ; in the hypoxic phase ( $h_2 < h < h_1$ ),  $\varphi_z = (h - h_1)/(h_2 - h_1)$ . The SWAP model allows  $h_3$  to vary as a function of potential transpiration rate ( $h_{3h}$  for high  $T_p$ , considered 5 mm d<sup>-1</sup>, and  $h_{3l}$  for low  $T_p$ , considered 1 mm d<sup>-1</sup>). In our study we adopted  $h_1=-10$  cm,  $h_2=-25$  cm,  $h_{3h}=-200$  cm,  $h_{3l}=-350$  cm and  $h_4=-5000$  cm, following the values proposed by (Taylor and Ashcroft, 1972).

Daily meteorological data of solar radiation (kJ m<sup>-2</sup>), maximum and minimum air temperature (°C), wind speed (m s<sup>-1</sup>) and relative humidity (%) and precipitation (mm) were collected at an automated weather station (geographic coordinates: 3°44'30"S 43°21'37"W) of

the Brazilian National Institute of Meteorology (INMET). In agreement to observed values, a rainfall intensity of 21 mm h<sup>-1</sup> was assumed in the SWAP scenarios.

A software routine developed by Pinheiro and de Jong van Lier, 2021 was used to run the SWAP model for each of the stochastic realizations and extracting the relevant water balance components (bottom flux, transpiration, evaporation, and runoff) from the SWAP output files.

#### 2.3. Results and Discussion

#### 2.3.1. Samples statistical properties

The stability test of the statistical properties as a function of the number of stochastic realizations for the three samples was confirmed through the corresponding root mean square error (RMSE) of means, standard errors, and correlation matrices.

We decided to use  $k = 10^5$ , corresponding to sufficiently small deviations from the original statistical properties of the sample. We considered the substantial gain in computational time with  $k = 10^5$  to outweigh the very small loss of accuracy when compared to  $k = 10^6$ . As we had three samples, 33,333 realizations for each replica were generated. Statistical properties of the merged dataset were calculated and used as the final result of the procedure.

Mean values, standard errors, and correlation matrices for the four VGM parameters  $\theta_s$ ,  $\alpha$ , n, and 1 obtained from the Hydrus inverse modelling output are shown in Table 1 for each of the three samples. Correlation matrices as they appear in this and following tables are the result of an empirical analysis of the fitting or inverse modelling software and we used them to generate stochastic realizations. Implicitly, a correlation between parameters reduces their independency. For example, in Table 1 a very high correlation is observed between  $\theta_s$  and  $\alpha$  in samples S1 and S3, and corresponding stochastic realizations will therefore show the same high correlation.

Table 1. Means, standard errors, and correlation matrices for the VGM parameters  $\theta_s$ ,  $\alpha$ , n, and l obtained from the Hydrus inverse modelling output for each sample.

-		<u> </u>						
Sample	Parameter	nrameter Mean Star	Standard error	Correlation Matrix				
	Turumeter		Standard error	$\theta_s$	α	n	1	
S1	$\theta_{\rm s}$	0.4853	0.0666	1				
	$\alpha$ (cm <sup>-1</sup> )	0.0615	0.0331	0.9900	1			
51	n	1.9476	0.5000	-0.7302	-0.8063	1		
	1	1.4987	1.2664	-0.8744	-0.8658	0.6724	1	
S2	$\theta_{\rm s}$	0.4725	0.0385	1				
	$\alpha$ (cm <sup>-1</sup> )	0.0897	0.0183	0.6998	1			
52	n	1.8001	0.2896	0.4766	-0.2711	1		
	1	0.1462	0.5380	0.3648	0.0577	0.4515	1	
	$\theta_{s}$	0.4151	0.0358	1				
S3	$\alpha$ (cm <sup>-1</sup> )	0.0590	0.0253	0.9666	1			
33	n	1.5098	0.1439	0.7542	0.6022	1		
	1	0.0727	0.2902	0.0868	-0.2304	0.4086	1	

Table 2 shows values obtained (1) from 33,333 stochastic realizations for each individual sample; (2) for the merged dataset based on the merged  $k = 10^5$  realizations; and (3) from the  $k = 10^5$  stochastic realizations generated from the merged properties. Fig. 1 shows the water retention  $(\theta-h)$  and hydraulic conductivity (K-h) and  $K-\theta$ 0 curves of the three individual sample parameters and for the merged parameters. In agreement with the coarse soil texture, the water content reduces to values below  $0.1 \text{ cm}^3 \text{ cm}^{-3}$  at a pressure head of about -100 cm. The K-h curves show a relatively high dispersion for the more negative values of h, due to the very high sensitivity of h to  $\theta$  in this range.

Table 2. (1) Means, standard errors, and correlation matrices for the VGM parameters as obtained from 33,333 stochastic realizations for each of the samples S1, S2 and S3; (2) for the merged dataset based on the merged  $k = 10^5$  realizations; and (3) from the  $k = 10^5$  realizations generated from the merged properties.

Comple	Parameter	Mean	Standard	d Correlation Matrix			
Sample			error	$\theta_s$	α	n	1
	$\theta_{\mathrm{s}}$	0.4853	0.0666	1			
S1	$\alpha$ (cm <sup>-1</sup> )	0.0615	0.0332	0.9899	1		
	n	1.9469	0.5025	-0.7306	-0.8070	1	
	1	1.5015	1.2700	-0.8738	-0.8653	0.6734	1
-	$\theta_{\rm s}$	0.4720	0.0386	1			
S2	$\alpha$ (cm <sup>-1</sup> )	0.0897	0.0183	0.7031	1		
32	n	1.7985	0.2891	0.4781	-0.2651	1	
	1	0.1472	0.5367	0.3610	0.0562	0.4493	1
S3	$\theta_{\rm s}$	0.4151	0.0359	1			
	$\alpha$ (cm <sup>-1</sup> )	0.0589	0.0255	0.9674	1		
	n	1.5104	0.1432	0.7538	0.6040	1	
	1	0.0738	0.2879	-0.0893	-0.2299	0.4048	1
M 114	$\theta_{\rm s}$	0.4575	0.0577	1			
	$\alpha$ (cm <sup>-1</sup> )	0.0700	0.0298	0.7917	1		
Merged dataset	n	1.7519	0.3895	0.0164	-0.3073	1	
	1	0.5742	1.0450	-0.1467	-0.5169	0.6534	1
Stochastic	$\theta_{s}$	0.4573	0.0577	1			
realizations from	$\alpha$ (cm <sup>-1</sup> )	0.0700	0.0299	0.7927	1		
	n	1.7523	0.3900	0.0159	-0.3072	1	
merged parameters	1	0.5737	1.0465	-0.1485	-0.5187	0.6526	1

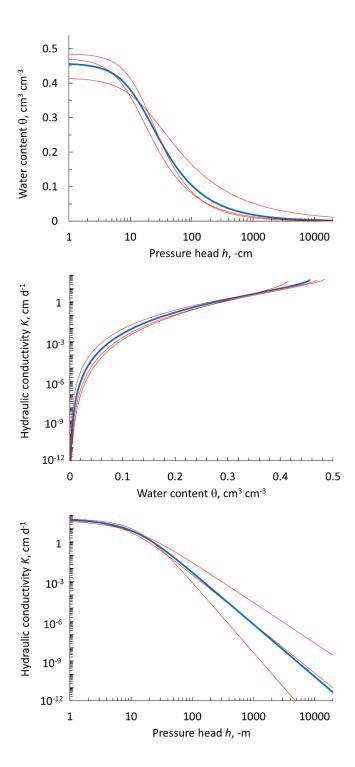


Fig. 1. Average water retention  $(\theta-h)$  and hydraulic conductivity (K-h) and  $K-\theta$  curves of the three individual sample parameters (red lines) and for the merged parameters (blue line).

Relatively high standard errors may result in the generation of stochastic realizations with parameter values outside the physically allowed range. Explicit parameter restrictions for the van Genuchten, (1980) equation with Mualem, (1976) restriction are  $\alpha > 0$  and n > 1. Besides these, Durner et al., (1999) and de Jong Van Lier et al., (2009) showed that, to guarantee  $dD/d\theta > 0$  (with diffusivity  $D = K \, dh/d\theta$ ), the following additional restriction applies: l > n / (1-n). We checked for these restrictions in the generated datasets, and a very small part of the realizations (less than 0.5%) did not comply and was eliminated.

#### 2.3.2. Level 1 comparison – individual parameter values

Based on the statistical properties of the parameter values for the individual samples listed in Table 1, 33,333 stochastic realizations were generated for each of the samples S1, S2, and S3. The statistical properties of these sets or realizations are shown in Table 2, and as expected show high similarity to the original values in Table 1. Table 2 also shows the statistical properties of the merged (joint) dataset and the  $k = 10^5$  realizations generated from the merged properties.

Parameter realizations from the merged dataset are implicitly normally distributed, whereas the distribution of the realizations of the individual samples is a summation of three normal distributions (Fig. 2). Peaks corresponding to each sample can be more clearly identified in the case of smaller standard errors, as is the case for l and n parameters of sample S3, causing a higher concentration of values near the mean. In these cases, especially, the merged frequency distribution differs significantly from the individual sample distribution.

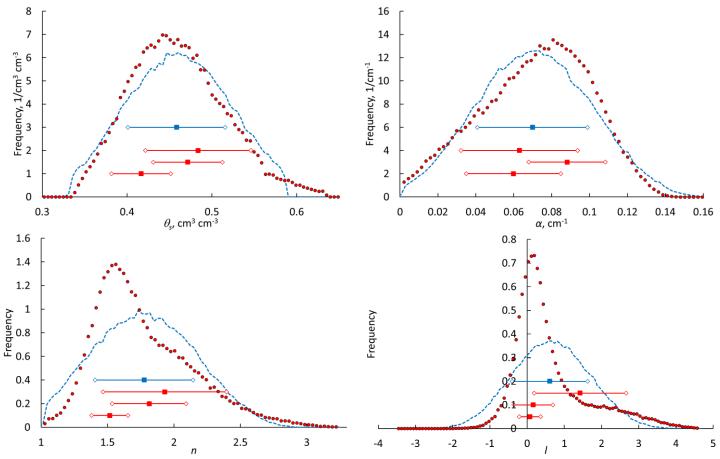
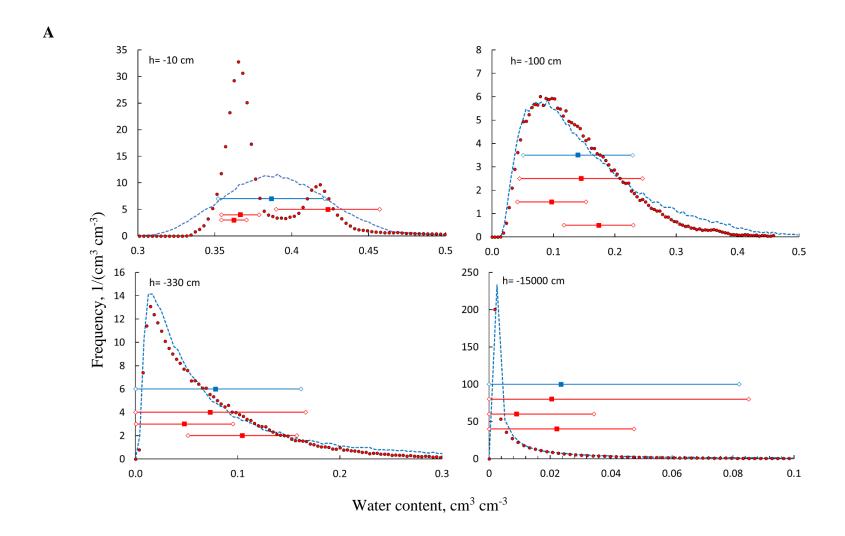


Fig. 2. Frequency distribution of VGM parameters for the sum of the realizations of three individual samples (3 x 33,333 realizations, red dots) and for the realizations with merged properties (100.000 realizations, blue dashed line). Horizontal lines represent mean and standard error of the merged dataset (blue) and individual samples (red).

#### **2.3.3.** Level 2 comparison – $\theta$ and K at specific pressure heads

The second level of comparison refers to the outcomes ( $\theta$  and K) of Eqs. 1 and 2 evaluated at specific pressure heads for each of the stochastic realizations of individual samples and of the merged parameter set. Figs. 3A and 3B show the corresponding frequency distributions of  $\theta$  and K at pressure heads of -10 cm, -100 cm, -330 cm, and -15000 cm. The distributions for the merged dataset differ from the sum of the individual samples, especially at the -10 cm tension.

The distributions at h = -10 cm are quite different from those for the saturated water content ( $\theta_s$ ) observed at level 1, although the water content at -10 cm is close to saturation. The individual sample maxima at h = -10 cm are not seen in  $\theta_s$ , showing that the other VGM parameters ( $\alpha$  and n) affected this result. However, as the tensions increase, individual sample peaks become imperceptible. Finally, at -15000 cm pressure head, the water content gets close to  $\theta_r$  which was assumed equal to zero.



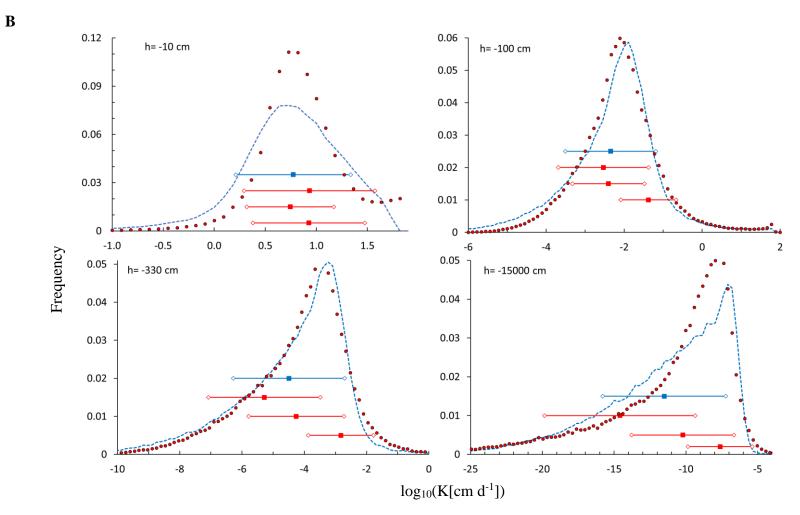


Fig. 3. Frequency distribution of water content (A) and hydraulic conductivity (B) at pressure heads -10 cm, -100 cm, -330 cm and -15000 cm for the sum of the realizations of three individual samples (3 x 33,333 realizations, red dots) and for the realizations with merged properties (100.000 realizations, blue dashed line). Horizontal lines represent mean and standard error of the merged dataset (blue) and individual samples (red).

#### 2.3.4. Level 3 comparison – soil water balance components

The third level of the evaluation was performed using outputs of the hydrological model SWAP for each of the k parameter realizations. This is, in fact, the most interesting and important level of evaluation, as soil hydraulic parameters are mainly determined to be used in models to perform simulations. To run a complete set of  $10^5$  simulations took about 48 h on an Intel Core i7 personal computer.

Whereas the water balance components bottom flux and runoff show a monomodal and slightly skewed distribution (Fig. 4), evaporation and transpiration are very asymmetrically distributed. Besides the distributions, Fig. 4 also shows those VGM parameters that presented a tendency as a function of the simulated values of water balance components. Parameters are shown in a normalized (0-1) format and were calculated as moving means with a window size of 4000 (out of 100.000) observations.

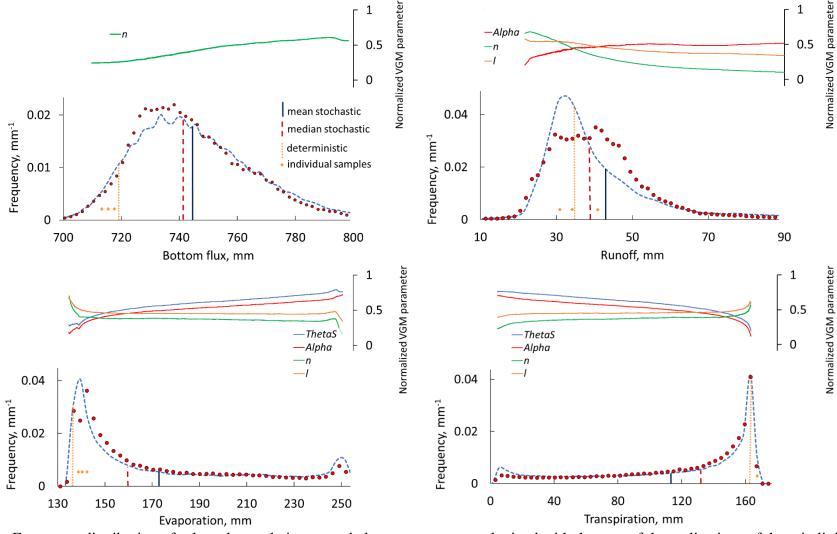


Fig. 4. Frequency distribution of selected cumulative water balance components obtained with the sum of the realizations of three individual samples (3 x 33,333 realizations, red dots) and with the realizations of merged properties (100.000 realizations, blue dashed line).

It is not so simple to give straightforward reasons for parameter tendencies as revealed in Fig. 4. In terms of the VGM equations, parameter l only affects the hydraulic conductivity function, and a higher l makes the value of K decrease faster with decreasing  $\theta$  or h. Parameter n affects both  $\theta$ –h and K- $(\theta,h)$ , where a higher n results in a steeper  $\theta$ -h curve and a higher  $\theta$  corresponding to a certain h, except for near-saturated conditions where  $\theta(h)$  becomes lower. An increase of n has the opposite effect on K- $\theta$  as an increase of l, making k decrease slower with decreasing  $\theta$ , however, due to the simultaneous effect of n on  $\theta(h)$ , a higher n will make K(h) decrease faster with decreasing h. Parameter  $\alpha$  affects the  $\theta(h)$  and K(h) relations, and a greater  $\alpha$  makes the  $\theta$  and K corresponding to a certain h to increase.

For bottom flux, the only significant correlation with VGM parameters was a positive one with parameter n (Fig. 4). The precise reasons for this are unclear. Bottom flux results from the internal drainage of water. A higher bottom flux is expected when more water infiltrates, corresponding to a lower runoff, which correlates to a higher  $K_s$  and lower surface layer water contents. It is also correlated to lower evapotranspiration rates. Transpiration may be reduced by the Feddes function as a function of pressure head h. A high transpiration rate may result in a drier surface layer with less evaporation and a higher sorptivity, hence a higher infiltrability. In fact, only a numerical model can disentangle all these interacting factors to result in the bottom flux from Fig. 4. The mean value of bottom flux (746 mm) represented 64% of the rainfall, which contributed to the mean runoff values being relatively low (44 mm), representing less than 4% of the mean observed rain.

Regarding transpiration and evaporation, the SWAP model considers potential evapotranspiration to be partitioned into potential transpiration ( $T_p$ ) and potential evaporation ( $E_p$ ),  $E_p$  being a negative exponential function of the leaf area index (LAI) or soil cover fraction.  $T_a$  may be lower than  $T_p$  as a function of profile pressure heads according to the reduction function proposed by Feddes et al., (1978), and actual evaporation ( $E_a$ ) may be smaller than  $E_p$  in the case of a low surface layer water content. A transpiration reduction ( $T_a < T_p$ ) also translates into a reduction in dry matter accumulation, hence a slower increase in LAI, which will affect the partitioning between  $E_p$  and  $T_p$  in the subsequent simulation time step. This feedback, besides the further dependency of  $E_a$  and  $T_a$  on the entire soil water balance, shows that a direct causal relationship between VGM parameters and simulated evapotranspiration will probably not exist. In our simulations, the maximum simulated cumulative transpiration was close to the maximum cumulative  $T_p$  of 165.2 mm, but some parameter combinations resulted in much lower values, down to 0 mm. High values of

cumulative transpiration corresponded to scenarios with higher  $\theta_s$  and  $\alpha$  and lower n and l, which both contribute to a slower decrease of K(h) with decreasing h.

For the case of evaporation, the trends were opposite, which is explained by the inverse impact of LAI on transpiration and evaporation. Furthermore, the scenarios with low transpiration due to crop water stress resulted in a proportionally lower LAI, favouring evaporation.

Fig. 4 also shows the mean of the stochastic realizations and the deterministic values for each water balance component. By comparing the two values of each component a significant difference is found, which demonstrates that not including uncertainties in the merging process may generate unrepresentative results.

Overall, considering the results at this third level of comparison, the merging method proved to be efficient for the simulated scenario. Despite the observed differences at levels 1 and 2, simulated distributions of water balance components are similar for the individual samples and the merged dataset. The effectiveness of the method in other scenarios (different soils, climate, and/or crops) would need more investigation, although there are no reasons to believe that results would be very different.

Finally, why would someone opt for the merging approach if the use of individual sample values results in similar results and distributions? The reason lies in practical aspects like reporting and modelling. A single (merged) parameter set is of course preferable over several individual sample data. This practice of merging is, in fact, very common when reporting soil property information by taking mean and standard deviation. Our proposal, for soil hydraulic parameters, implies in an enhanced method to do so including a stochastic interpretation.

#### 2.4. Conclusions

We presented a method for merging soil hydraulic parameters using stochastic realizations of van Genuchten-Mualem parameters generated by Cholesky decomposition. The method of stochastic merging proved to correctly represent the variability of the combined replicas, especially when used in a hydrological model to predict soil water balance components. From this, we conclude that:

i) Applying the proposed method to obtain merged parameters, the frequency distribution of predicted water balance components evaporation, transpiration,

- bottom flux, and runoff are very similar using the merged or the individual parameters;
- ii) The values of the predicted water balance components using mean hydraulic property parameter values are substantially different than the mean values of stochastic realizations using the merged parameter set, indicating that the common practice of deterministic modelling with mean values may bias final results and showing the importance of stochastic analyses.

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# 3. STOCHASTIC ASSESSMENT OF SOIL WATER BALANCE COMPONENTS IN A HARDSETTING SOIL SCENARIO

### **Abstract**

Hardsetting soils have a natural densification that confers to the soil a low total porosity, resulting in problems related to water flow. Evaluating the water balance components in vadose zone of systems in soils like the one in this study, allows us to characterize and understand the processes related to the soil water flow. To this end, hydrological modelling presents itself as a useful tool, since it is possible to understand, based on historical series, the behaviour of these processes over time. The use of hydrological models is based on parameters of soil water retention and hydraulic conductivity – normally determined through different replicas of soil samples. However, when the objective is to represent large areas, this method may not be the most effective, since it works with the average of the replicas. Based on this, a method was used to merge the soil hydraulic parameters of all replicas into a single dataset, with their associated statistics (standard errors and correlation matrix). Based on this, this work aimed to evaluate the water balance components (bottom flux, evaporation, transpiration, and runoff) over a 31-year period in a hardsetting soil cultivated with a soybeanmillet rotation in the eastern region of Maranhão state, Brazil. To do so, van Genuchten-Mualem (VGM) parameters of three replicas collected at three soil depths (0-15, 15-30, and 30-45 cm) were used, comparing the use of stochastic medians values with the deterministic mean values. Applying the stochastic technique, some generated VGM parameter sets, as well as the rainfall accumulation and distribution during the crop cycle, proved to be the determining factors for the dispersion of the water balance components results. Except for transpiration, the other water balance components showed a good correlation with the accumulated rainfall. A significant reduction in transpiration rate was noticed in years with high precipitation. Overall, using the mean hydraulic parameter values to deterministically predict water balance components can produce outputs that are substantially different from the median stochastic values. This suggests that deterministic modelling may generate results that do not represent the parameters with their uncertainties and correlations.

Keywords: Hardsetting soil; Soil sampling; Stochastic method; Soil water retention; hydraulic conductivity; Water balance components.

## 3.1. Introduction

Globally, hardsetting soils occur in arid, semi-arid, and Mediterranean tropical regions (Mullins 1999). It is a common soil type in regions with an alternation of dry and humid periods. In Brazil, hardsetting soils are found mainly in the Coastal Tablelands in the Southeast and Northeast of Brazil, occupying about 200.000 km². The diagnostic attribute "hardsetting character" is described in the Brazilian Soil Classification System (Embrapa 2013)(Embrapa 2013) as a pedogenetic characteristic (densification) in the subsurface horizons (BA, Bw, or Bt), with medium, clayey or very clayey texture, usually found between 30 and 70 cm depth. The last definition was made by (McDonald and Isbell 2009) and includes the concepts of apedality and reversibility: 'Compact, hard, apparently apedal condition forms on drying but softens on wetting'.

A portion of Brazil's hardsetting soils is found in the Cerrado biome, since the Coastal Tablelands cover part of Piauí and Maranhão states, where, respectively, about 46 and 60% are occupied by Cerrado (FUNDAÇÃO CEPRO 2014; IMESC 2020). The Cerrado (Brazilian savannah) is the second largest biome in Brazil, with less than 1% of its area preserved. In contrast, more than 50% of the biome (approximately 2 million km²) has been converted to pasture and agricultural land in recent decades (Beuchle et al. 2015; Klink and Machado 2005). This has characterized the Cerrado as the most important biome for agricultural expansion in the country. The eastern region of the state is one of the most productive agricultural frontiers (Schlesinger et al. 2008), with emphasis on soybean cropping. However, there is a great difficulty in increasing soybean yield grown in hardsetting soils mainly due to the reduced soil macroporosity. Due to problems such as deficient aeration and low macroporosity, hardsetting soils present serious problems related to root penetration (Cintra et al. 2004) and water flow (Fabíola et al. 2002), determining factors for crop productivity.

In addition to all the problems inherent to the soil, after the rainy season in the study region (January to June), the accumulated rainfall is very low and the average temperatures higher, which is a limiting factor for crop production in a non-irrigated system. With this scenario, most producers harvest only one soybean crop per year (during the rainy season), and they try to grow a millet crop to generate soil organic matter. However, since this crop is grown during the dry period, a low amount of dry matter is generated. In addition, since the rate of decomposition has a direct relationship with high temperatures and precipitation (Vivanco and Austin 2019), the decomposition rate in the study region is very low.

In that context, the objective of this research was to evaluate the water balance components for a 31-year period in a hardsetting soil cultivated with soybean-millet rotation in the eastern region of the state of Maranhão, Brazil. To allow an uncertainty analysis, the methodology proposed by Santos et al., 2022 for merging the soil hydraulic properties (SHP) and the associated statistics of several soil samples into a single set of parameters was used. Simulations with each stochastic realization of SHP were performed and the outcome and uncertainty of simulated water balance components were evaluated.

#### 3.2. Material and Methods

# 3.2.1. Sampling information

Undisturbed soil samples (height 7 cm; internal diameter 7.4 cm) were collected in three soil depth (0-15, 15-30 and 30-45 cm depth) of soybean/millet area of the Brazilian

savanna in Maranhão State, Brazil (3°16'59"S 43°28'52"W) (Fig. 1). The soil is classified as a Haplic Acrisol (IUSS Working Group WRB-FAO, 2015) with loamy sand texture (0.819 kg kg<sup>-1</sup> sand, 0.055 kg kg<sup>-1</sup> silt, and 0.126 kg kg<sup>-1</sup> clay). The sampling location has a Koeppen Aw climate (Tropical savanna climate with dry-winter characteristics) with an annual rainfall of 1670 mm and a mean temperature of 27 °C. Annual, monthly precipitation and average temperature are presented in Fig. 2 and 3.

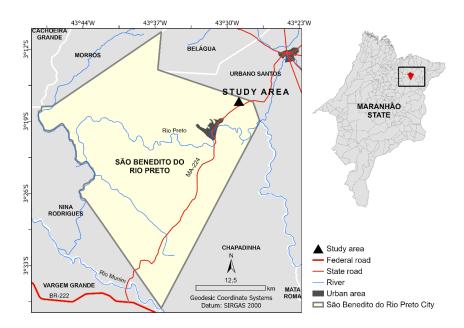


Fig. 1. Geographic location of the study area.

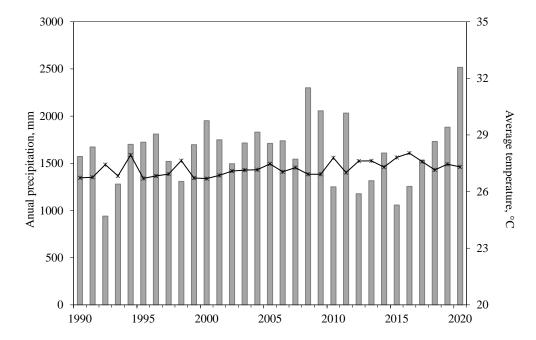


Fig. 2. Annual rainfall (bars) and average annual temperature (line) of the study region for a 31-year period (1990 to 2020). Source: INMET.

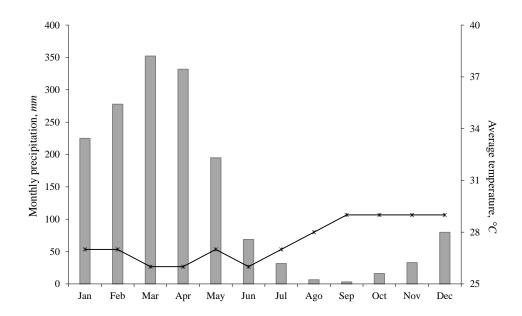


Fig. 3. Monthly rainfall (bars) and average annual temperature (line) of the study region for a 31-year period (1990 to 2020). Source: INMET.

# 3.2.2. Soil hydraulic properties

The soil hydraulic properties are described by the van Genuchten-Mualem (VGM) analytical K- $\theta$ -h functions (van Genuchten 1980; Mualem 1976):

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[ 1 + \left( \alpha |h| \right)^n \right]^{\frac{1}{n} - 1}$$
(5)

$$K = K_{sat} \Theta' \left[ 1 - \left( 1 - \Theta^{\frac{n}{n-1}} \right)^{1 - \frac{1}{n}} \right]^2$$
 (6)

where  $\Theta$  is the effective saturation,  $\theta$  (cm<sup>3</sup> cm<sup>-3</sup>) is the volumetric water content, h (cm) is the pressure head, and K (cm d<sup>-1</sup>) is the unsaturated hydraulic conductivity. In these equations, six parameters define the soil hydraulic properties and will be referred to as the van Genuchten-Mualem (VGM) parameters:  $\theta_r$  (residual water content, cm<sup>3</sup> cm<sup>-3</sup>),  $\theta_s$  (saturated water content, cm<sup>3</sup> cm<sup>-3</sup>),  $K_s$  (saturated hydraulic conductivity, cm d<sup>-1</sup>), and shape parameters  $\alpha$  (cm<sup>-1</sup>), n (-), and l (-).

## 3.2.3. Obtaining a set of VGM parameters

The VGM parameters were obtained from an evaporation experiment with the undisturbed soil samples. Soil samples were saturated by capillary rise from the bottom for 48 h. Subsequently, repeated measurements of gamma-ray attenuation and sample weight were made every 24 h until negligible weight change (< 1 g d<sup>-1</sup> equivalent to < 0.01 m<sup>3</sup> m<sup>-3</sup> d<sup>-1</sup>). The samples were weighed, and the water content was measured by gamma-ray attenuation using a 3 mm diameter collimated <sup>137</sup>Cs beam. Readings were made twice at each of five vertical positions in the sample: 1.0, 1.5, 2.0, 3.5, and 5.0 cm below the sample surface. The counting time was 20 s for each reading. Subsequently, the sample was kept in the laboratory to evaporate from the upper surface, with a controlled temperature between 18 and 21 °C. At the end of the experiment, the final water content was determined by oven drying at 105 °C for 24 h and a final gamma reading in the oven-dry sample was performed. The evaporation rate between subsequent series of measurements was determined by weight difference. Attenuation readings were transformed to water content using the Beer-Lambert attenuation law (Wang et al. 1975) together with the attenuation coefficient of pure water and the soil particles, determined from the final oven-dry reading.

The inverse modelling option of Hydrus-1D (Šimůnek et al. 2016) was used to obtain the hydraulic parameters and associated statistics for each sample. Hydrus-1D simulates one-dimensional variable-saturated water flow in porous media by numerically solving the Richards equation. The Marquardt-Levenberg algorithm is used for inverse problem

optimization. The boundary conditions were set to reflect the measured evaporation flux at the upper boundary and a zero flux at the lower boundary.

Measured water contents over depth and time together with measured evaporation rates were used to compose the objective function to be minimized by Hydrus-1D. As a result, Hydrus produces an estimate of the parameters from Eqs. [1] and [2] as well as respective standard errors and correlation matrix. To reduce the uncertainties of the parameter estimates, fixed values of  $\theta_r = 0$  and l = 0.5 were used.  $K_s$  values were determined based on studies carried out with soils like the one used in this study (Santos 2018; Silva 2019).  $\theta_r$  was fixed at this value because, in all simulations, its value converged to zero, and the used value of  $K_s$  (15.0, 7.2 and 3.0 for 0-15, 15-30 and 30-45 cm soil depth, respectively) corresponds to measurements performed in soils from the region. The remaining four parameters ( $\theta_s$ ,  $\alpha$ , n) were obtained by the inverse modelling.

## 3.2.4. Merging statistical properties of hydraulic parameters from replicas

To merge the statistical properties of three replicas into one set of information (merged means, standard errors, and correlation matrix) while preserving the properties of the individual replicas, stochastic realizations of the parameter set for each sample were generated. These sets of realizations of all the replicas were joined together and the properties of the resulting merged dataset were calculated.

To merge the replicas, the methodology proposed by Santos et al., 2022 was used. To remove outliers and negative values, a tail fraction  $(\tau)$  of 0.03 was applied.

## 3.2.5. Agro-hydrological simulations

The water balance components (WBC) were simulated for a 31-year period (1990 to 2020) using the agro-hydrological model SWAP-1D, version 4.2.0 (Kroes et al. 2017). The simulations were performed using stochastic realizations from the merged sample properties (Table 1). A software routine developed by Pinheiro and de Jong van Lier, 2021 was used to run the SWAP model for each of the stochastic realizations and extracting the relevant WBC components bottom flux, evaporation, transpiration, and runoff) from the output files.

In this study,  $10^4$  stochastic realizations were generated. Corresponding  $10^4$  simulations took about 72 h on an Intel Core i7 personal computer. To identify whether all

stochastic realizations generated for the WBC had a normal distribution, a Kolmogorov-Smirnov test was performed, at a significance level of  $\alpha = 0.05$ .

SWAP employs a discretized form of the Richards equation (van Dam and Feddes 2000) including a root water extraction sink term, according to:

$$C(h)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z} \left[ K(h) \left( \frac{\partial h}{\partial z} + 1 \right) \right] - S(h)$$
 (3)

where C(h) is the differential water capacity  $(\partial\theta/\partial h, [\text{cm}^{-1}])$ , t is time [d], z is the vertical coordinate taken positive upwards [cm], h is the pressure head [cm], K(h) is the hydraulic conductivity [cm d<sup>-1</sup>] and S(h) represents water uptake by plant roots [d<sup>-1</sup>]. The numerical solution of Eq. (5) requires parameterizing the unsaturated soil hydraulic properties  $(K-\theta-h)$ , here described by the analytical functions from the van Genuchten-Mualem model [Eqs. (1) and (2)].

The outputs include cumulative WBC bottom flux, transpiration, evaporation, and runoff. These were simulated for a rainfed soybean scenario using a crop cycle of 120 days and a millet crop cycle of 90 days with a maximum rooting depth of 0.75 m.

A soil profile depth of 1.5 m was used in the simulations. The bottom boundary condition was set to free drainage (gravitational flow) and the upper boundary condition was described in terms of potential evapotranspiration ( $ET_p$ ) based on direct application of Penman-Monteith and precipitation. The SWAP model partitions  $ET_p$  further into potential transpiration ( $T_p$ ) and potential evaporation ( $T_p$ ) according to the leaf area index.

When integrated over depth, the root water uptake term S(h) in Eq. (4) corresponds to the actual transpiration ( $T_a$  [cm d<sup>-1</sup>]) which is calculated according to a modified version of the transpiration reduction function proposed by Feddes et al., (1978).  $T_a$  [cm d<sup>-1</sup>] is calculated by multiplying the potential transpiration  $T_p$  [cm d<sup>-1</sup>] by an empirical factor  $\varphi_z$ , evaluated for each soil layer (z) and weighted by the layer thickness  $w_z$  [L] and the relative root length density in the respective layer ( $R_z$ ):

$$T_{a} = T_{\rho} \frac{\sum_{z=1}^{z} \left[ \varphi_{z} \mathbf{w}_{z} R_{z} \right]}{\sum_{z=1}^{z} \mathbf{w}_{z} R_{z}}$$

$$\tag{4}$$

The empirical reduction factor  $\varphi_z$  ( $0 \le \varphi_z \le 1$ ) is defined by four threshold pressure head values ( $h_4 < h_3 < h_2 < h_1 \le 0$ ). Below wilting point ( $h < h_4$ ) and in the anoxic phase ( $h > h_1$ ),  $\varphi_z = 0$ ; in the falling rate phase ( $h_4 < h < h_3$ ),  $\varphi_z = (h - h_4)/(h_3 - h_4)$ ; in the constant (optimum) rate, delimited by  $h_3$  and  $h_2$ ,  $\varphi_z = 1$ ; in the hypoxic phase ( $h_2 < h < h_1$ ),  $\varphi_z = (h - h_1)/(h_2 - h_1)$ .

The SWAP model allows  $h_3$  to vary as a function of potential transpiration rate ( $h_{3h}$  for high  $T_p$ , considered 5 mm d<sup>-1</sup>, and  $h_{3l}$  for low  $T_p$ , considered 1 mm d<sup>-1</sup>). In our study we adopted  $h_1$ =-10 cm,  $h_2$ =-25 cm,  $h_{3h}$ = -200 cm,  $h_{3l}$ = -350 cm and  $h_4$  = -5000 cm, following the values proposed by (Taylor and Ashcroft 1972).

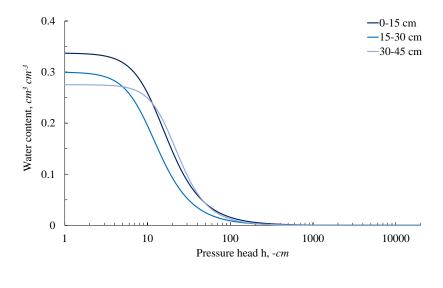
Daily meteorological data of solar radiation (kJ m<sup>-2</sup>), maximum and minimum air temperature (°C), wind speed (m s<sup>-1</sup>) and relative humidity (%) and precipitation (mm) were collected at an automated weather station (geographic coordinates: 3°44′30″S 43°21′37″W) of the Brazilian National Institute of Meteorology (INMET). In agreement to observed values, a rainfall intensity of 21 mm h<sup>-1</sup> was assumed in the SWAP scenarios.

Detailed information about soil and crop parameters used in the simulations are listed in appendices A, B and C.

# 3.3. Results and Discussion

## 3.3.1. Soil water retention and hydraulic conductivity

Fig. 4 shows the water retention  $(\theta-h)$  and hydraulic conductivity (K-h) curves of the merged parameters for the three soil depths (0-15, 15-30 and 30-45 cm) used for the 31-year simulations (1990 to 2020). Since the soil of the study region is very sandy, the water content reduces to values below  $0.1 \text{ cm}^3 \text{ cm}^{-3}$  at a pressure head of about -100 cm at all soil depths. Due to the high dependence on  $\theta$ , the hydraulic conductivity showed the same behaviour, with higher values in the 0-15 cm depth and decreasing for the underlying depths.



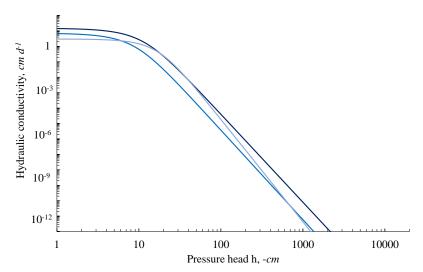


Fig. 4. Water retention  $(\theta-h)$  and hydraulic conductivity (K-h) functions for the three depths (0-15, 15-30 and 30-45 cm) in the studied soil.

Table 1 shows the VGM parameters and their standard errors for the three soil depths used in the simulations and in Table 2 the corresponding correlation coefficients are presented.

<b>Table 1.</b> van Genuchten-Mualem parameters for the three soil depths used in this study. The
values between parentheses are the respective standard errors.

Depth (cm)	$\theta_r$	$\theta_s$	α	n	$K_s$	l
	cn	n <sup>3</sup> cm <sup>-3</sup>	cm <sup>-1</sup>	-	cm d <sup>-1</sup>	-
0-15	0.0	0.3374	0.0792	2.4809	15.0	0.5
	0.0	(0.0223)	(0.0197)	(0.5419)	13.0	0.3
15-30	0.0	0.3001	0.1018	2.5206	7.2	0.5
	0.0	(0.0123)	(0.0378)	(0.6216)	1.2	0.5
30-45	0.0	0.2753	0.0535	2.8546	3.0	0.5
	0.0	(0.0140)	(0.0150)	(0.6251)	3.0	0.3

**Table 2.** Parameter correlation matrices obtained from Hydrus-1D inverse modelling of laboratory evaporation experiments.

Depth (cm)	Domomoton -	Correlation Matrix						
	Parameter -	$\theta_{ m s}$	α	n				
	$\theta_{ m s}$	1		_				
0-15	α	-0.0359	1					
	n	0.2492	0.7934	1				
	$\Theta_{ m s}$	1						
15-30	α	-0.1290	1					
	n	-0.3628	-0.8096	1				
30-45	$\Theta_{ m s}$	1						
	α	0.5712	1					
	n	-0.7897	-0.1877	1				

# 3.3.2. Water balance components (WBC)

The WBC bottom flux, transpiration, evaporation, and runoff showed a wide variation over the 31-year period, depending on the accumulated rainfall and the rainfall distribution throughout the soybean crop cycle. These results are shown in Figs. 5a to 5d. Table 3 shows the deterministic mean values of the WBCs and the medians of the stochastic values, both with their respective means and standard deviation. In Table 4 shows are presented the annual average water balance components for the 31-year period (31 values) and for all 10<sup>4</sup> values of all years combined (31·10<sup>4</sup> values): 5 and 95% percentiles, median, standard deviation (SD) and and coefficient of variation (CV). With the exception of evaporation, all WBCs showed a high CV, which demonstrates that, in general, there was a large dispersion of data around the median value. In the next sections, the results generated from the 31·10<sup>4</sup> stochastic realizations will be considered.

To check whether the stochastic performances of the WBCs were normal or not, the Kolmogorov-Smirnov test was applied, with a significance level of  $\alpha=0.05$ . The test showed, for all WBCs, in all years, that the data were not normal. Due to this result, we will report the median in this work.

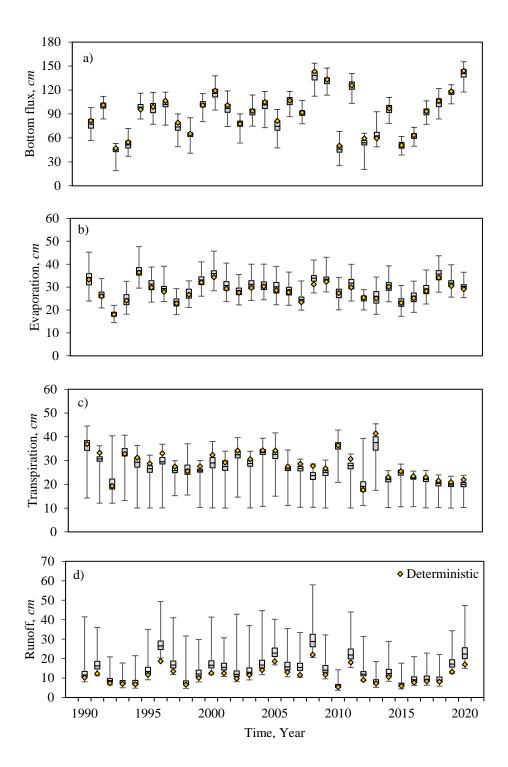


Fig. 5. Box plot graphs of stochastic simulations of water balance components for the 31-year period (1990 to 2020) with soybean and millet crops in the study region. a)

Bottom flux; b) Evaporation; c) Transpiration; d) Runoff.

**Table 3.** Deterministic mean values of the WBCs and the medians of the stochastic values for 1990 to 2020. *T*, *E*, *BF*, and *R* stand for transpiration, evaporation, bottom flux, and runoff, respectively.

Year -	BF, c	BF, cm		E, cm		ı	R, cn	R, cm	
	Det.	Stoch.	Det.	Stoch.	Det.	Stoch.	Det.	Stoch.	
1990	81.5	77.3	33.3	34.2	36.9	36.5	10.2	11.6	
1991	101.0	100.4	26.0	26.8	33.2	30.7	12.3	16.3	
1992	47.0	45.3	18.1	18.4	19.3	20.0	7.3	8.7	
1993	54.6	51.3	24.1	24.7	32.8	33.4	7.0	7.5	
1994	95.4	98.6	36.4	37.1	31.2	29.3	6.8	7.3	
1995	98.9	97.4	29.8	31.3	28.7	26.6	11.6	13.3	
1996	106.4	102.0	27.9	29.3	33.0	29.5	18.6	26.5	
1997	79.0	73.9	22.9	23.7	27.4	25.8	13.4	16.7	
1998	65.3	64.1	26.7	27.3	25.5	26.2	6.6	7.2	
1999	100.9	102.7	32.0	33.1	27.5	25.7	10.0	12.1	
2000	119.2	115.7	34.3	35.9	32.3	29.0	12.5	16.6	
2001	100.9	97.0	29.3	30.7	29.2	27.5	12.4	15.5	
2002	77.4	77.6	27.6	28.5	34.2	32.5	9.7	11.9	
2003	93.8	92.5	29.6	31.2	30.5	28.8	11.5	13.0	
2004	104.9	101.6	30.3	31.1	34.2	33.5	14.0	16.7	
2005	81.2	74.6	28.6	30.2	34.2	32.6	18.5	22.9	
2006	106.7	106.1	27.7	28.9	27.5	26.6	13.0	15.8	
2007	91.6	91.1	23.4	24.6	28.6	26.7	11.6	15.5	
2008	143.3	138.1	31.2	33.9	27.7	23.7	21.9	28.8	
2009	133.0	131.6	32.3	33.5	26.7	25.0	11.7	14.1	
2010	50.1	46.0	27.4	27.9	36.4	36.5	5.3	5.6	
2011	125.7	125.5	29.8	31.7	30.7	27.9	18.0	21.9	
2012	59.5	54.0	25.4	25.5	17.6	19.1	8.9	12.0	
2013	59.3	62.6	25.0	25.9	41.3	37.6	7.2	7.8	
2014	97.0	96.1	30.2	30.9	23.0	22.1	10.5	12.3	
2015	50.9	50.5	23.1	23.6	25.5	25.1	5.9	6.4	
2016	63.3	62.2	25.2	26.0	23.4	22.6	7.6	9.2	
2017	93.3	92.3	28.2	29.2	23.0	22.1	8.3	9.3	
2018	106.3	103.9	34.1	35.7	21.5	20.4	8.0	8.8	
2019	118.4	117.1	30.5	31.8	20.9	19.8	13.2	17.2	
2020	144.1	140.8	29.1	30.4	21.9	20.0	16.9	22.4	
Mean	91.0	59.2	28.9	29.0	27.9	19.2	12.6	13.9	
SD	26.8	36.5	4.1	4.9	5.4	9.3	5.3	5.9	

**Table 4.** Annual average water balance components for 1990 to 2020: Minimum, maximum, percentiles 5 e 95%, median, standard deviation (SD) and coefficient of variation (CV) values of average of each year combined (31 values) and of all values with all years combined (31·10<sup>4</sup> values). T, E, BF, and R stand for transpiration, evaporation, bottom flux, and runoff, respectively.

-	Average of 31-year period				Averag	Average of 31-year period			
	(31 values)				(3	$31 \cdot 10^4$	values)		
WBC	BF	Е	T	R		BF	Е	T	R
Perc. 5%	48.6	23.2	19.7	7.3		46.3	21.0	18.5	6.2
Perc. 95%	134.5	35.5	36.2	25.4		136.2	36.6	36.7	27.3
Median	96.1	30.2	26.6	13.0		94.0	29.3	26.6	13.5
SD	26.8	4.2	5.1	6.0		26.9	4.7	5.6	6.6
CV (%) <sup>1</sup>	27.9	13.9	19.2	46.2		28.6	16.0	21.1	48.9

<sup>&</sup>lt;sup>1</sup>Thorndike's coefficient of variation (SD ÷ Median).

In general, based on Figs 5a to 5d and Table 3, using the mean VGM parameter values to predict the water balance components may generate results that are considerably different than the median values of stochastic realizations. Among the WBCs, bottom flux and transpiration presented the greatest difference between the deterministic mean values and the median values resulting from the stochastic realizations, mainly in high-rainfall years. Thus, a mere deterministic modelling result may not present itself as a good prediction tool for water balance components.

The bottom flux data (Fig. 5a) expressed the largest variation between the 5 and 95% percentiles (46.3 to 136.2), showing that this WBC was the one that most varied according to the variation of the generated VGM parameters and with the distribution and accumulated rainfall. This large variation is confirmed by the high standard deviation value (26.9 mm). The bottom flux data variance was directly proportional to the accumulated rainfall, and this trend was confirmed from the determination and correlation coefficients (Fig. 6), which were 0.91 and 95%, respectively. However, this does imply that all the rainwater infiltrates into the soil. In large precipitation events, some of the water will infiltrate and will be lost by evaporation, transpiration, and drainage (Kiehl, 1979). Due to the reduced porosity of the subsurface depths, hardsetting soils present a low hydraulic conductivity (Santana et al. 2006; Silva et al. 1998), which generates, in the presence of large precipitation events (with precipitation

greater than the infiltration velocity), a lower water entry into the soil profile and an increase in surface and subsurface runoff losses (Blanco-Canqui and Ruis 2018).

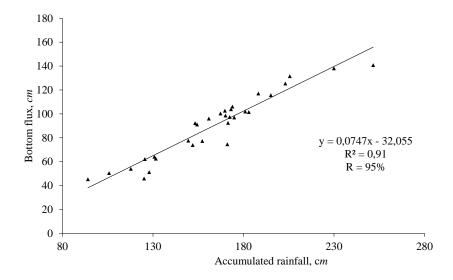


Fig. 6. Determination and correlation coefficients between accumulated rainfall and bottom flux for the 31-year period (1990 to 2020) for the studied soil and region.

In some years, the amplitude between the upper and lower limits of WBC was higher, especially in years with higher accumulated rainfall, where normally the rain distribution may not occur gradually during the crop cycle. The rainfall distribution over time is presented in Figs. 7 and 8. The year 2008 is a good example to illustrate, since it was one of the years with high rainfall resulting in a greater amplitude in the results. In this year (2008), in just two weeks it rained more than 550 mm, which represents more than 25% of the total rainfall for the whole year. Figs. 9 and 10 present the simulation results of pressure head and soil water content obtained with the mean hydraulic parameter values for 2008. Since the soil water content has a direct relationship with the pressure head (van Genuchten 1980), high values of soil moisture and pressure head were noted throughout the crop cycle.

On the other hand, when the crop received less water during the cycle, a smaller amplitude was observed in the values of bottom flux, evaporation, and transpiration. Figs. 11 and 12 show the results for the year 1992, in which rainfall occurred only during the first 90 days of the crop cycle, resulting in a period of water deficit of 30 days. This fact may have contributed to a decrease in the amplitude of WBC data this year.

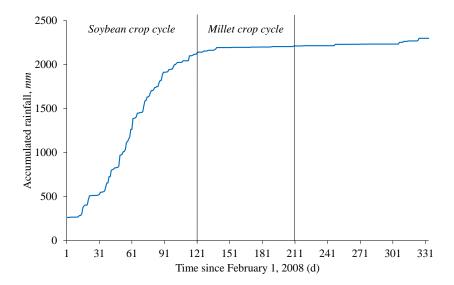


Fig. 7. Accumulated rainfall for the year 2008.

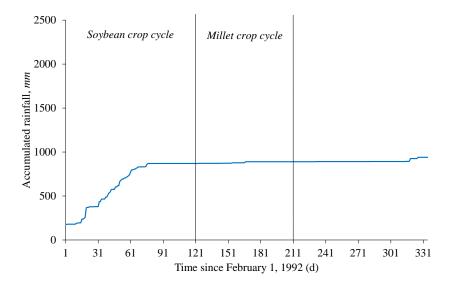


Fig. 8. Accumulated rainfall for the year 1992.

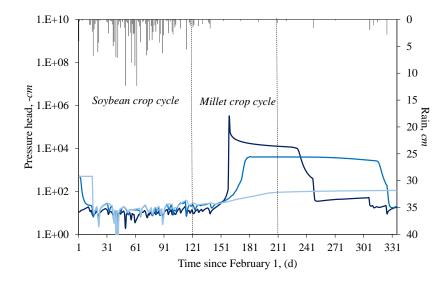


Fig. 9. Stochastic values of pressure head for 0-15, 15-30 and 30-45 cm depths during the year 2008 in the studied soil.

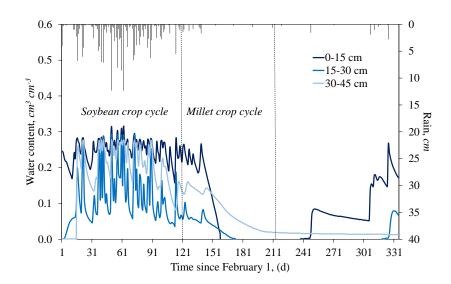


Fig. 10. Stochastic values of water content for 0-15, 15-30 and 30-45 cm depth during the year 2008 in the study region.

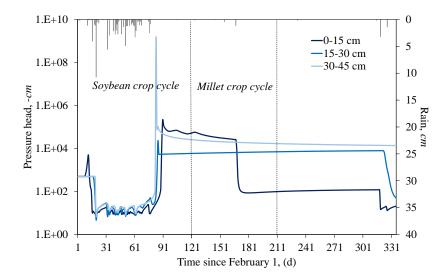


Fig. 11. Stochastic values of pressure head for 0-15, 15-30 and 30-45 cm depth during the year 1992 in the study region.

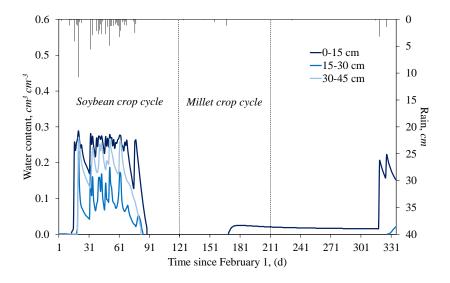


Fig. 12. Stochastic values of water content for 0-15, 15-30 and 30-45 cm depth during the year 1992 in the study region.

Regarding evaporation data (Fig. 4b), the trend was somehow different. The variation between the 5 and 95% percentiles was smaller (21.0 to 36.6 mm). As noticed for bottom flux, there was high correlation between accumulated rainfall and evaporation (Fig. 13). The coefficients of determination and correlation observed were 0.49 and 70%, respectively, i.e., most of the evaporation results are explained by the accumulated rainfall. However, other variables such as soil cover and leaf area index (LAI) also affect this result. Correlating the bottom flux data with evaporation, a good correlation was also observed, since both are highly

dependent on soil moisture. The coefficients of determination and correlation were 0.48 and 69%, respectively. In general, observing Fig. 2, years with less accumulated precipitation (e.g., 1990, 1992) correspond to lower amplitudes, considering the upper and the lower limit.

In addition, in the study region, evaporation rates tend to be higher, since the soils have low levels of organic matter and little vegetation cover, which act as a physical barrier, protecting soil from direct sunlight (van Donk et al. 2010); Santos et al., 2022) and, consequently, reducing water losses by evaporation.

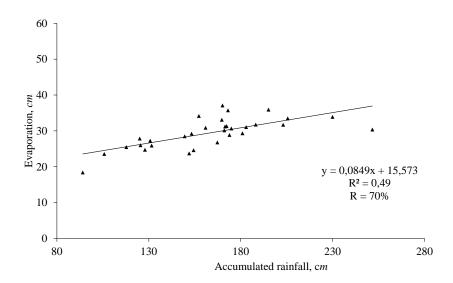


Fig. 13. Determination and correlation coefficients between accumulated rainfall and evaporation for the 31-year period (1990 to 2020) in the study region.

Unlike the previous results, transpiration values did not present a good correlation with the accumulated precipitation or with the other WBC. This fact is explained by the reduction in transpiration rates due to water deficit in the years with high accumulated rainfall. Noticing the transpiration rates for the years 2008 and 1992 (Figs. 14 and 15) the influence of rain on the transpiration reduction is observed. In general, dry climates with high vapour pressure deficits (as is the case for the study region) cause high transpiration rates to crops in the absence of drought stress. In years with less water availability, the temperature tends to increase, and this raises the vapour pressure gradient between the leaf and the atmospheric air, increasing the transpiration rate and the dry matter accumulation by crops (Hopkins et al. 1995). Additionally, low air humidity corresponding to lower rainfall amounts also increases the potential transpiration rate of crops (Song et al. 2021).

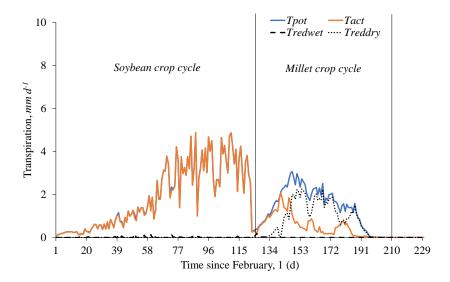


Fig. 14. Transpiration rates for the period with soybean and millet (February to September) in the year with the highest observed rainfall (2008).  $T_{pot}$ : potential transpiration;  $T_{act}$ : actual transpiration;  $T_{redwet}$ : reduction in transpiration due to water excess;  $T_{reddry}$ : reduction in transpiration due to water deficit.

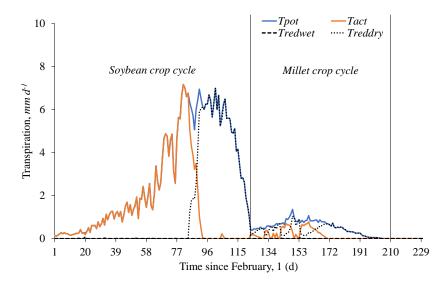


Fig. 15. Transpiration rates for the period with soybean and millet (February to September) in the year with the lowest observed rainfall (1992).  $T_{pot}$ : potential transpiration;  $T_{act}$ : actual transpiration;  $T_{redwet}$ : reduction in transpiration due to water excess;  $T_{reddry}$ : reduction in transpiration due to water deficit.

Considering the 5 and 95% percentiles, the transpiration varied between 18.5 and 36.7 mm in the soybean crop cycle. As shown in Fig. 5c, 50% of the values, represented by the distance between quartiles 1 and 3, were closer to the upper limit, which means that

transpiration values, in most years, tended to be higher. Few exceptions can be seen, as in the years 1992 and 2012, when the accumulated rainfall was slightly lower than the other years evaluated.

The runoff expressed the greatest dispersion of data around the median (CV 48.9%), which has high correlation with the large rainfall accumulation recorded in some years. Mainly in years with higher rainfall, runoff was higher, showing that there was a direct relation between the accumulated rainfall and this WBC. Observing the correlation and determination coefficients (0.56 and 75%, respectively) (Fig. 16), for the 31 years evaluated (1990 to 2020), this trend is confirmed. Fig. 5d shows that the highest runoff occurred in 2008. In this year, specifically, one of the highest values of accumulated rainfall was observed (2300 mm), whereas the climatic average is 1670 mm. Analysing the rainfall distribution over time (Fig. 7), it can be seen that, during the soybean crop cycle, the volume of rainfall was considerably larger (92% of the accumulated amount of the year). On average, it rained about 500 mm per month, which represents a much higher volume than commonly observed in the region, averaging 350 mm in March – the month with the highest rainfall (Fig. 3). On the other hand, in 1992 (Fig. 8), the amount of rain was roughly 50% of the 2008 rainfall, and it occurred during the first 90 days of the soybean crop cycle, resulting in a 30-day water deficit at the end of the crop cycle. As a result, 1992 was the year that presented the smallest variation in runoff values around the median.

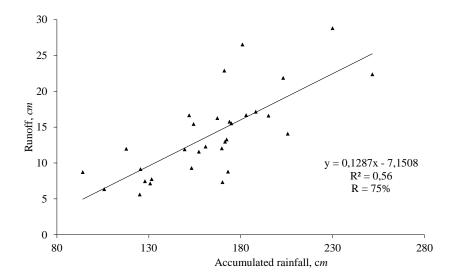


Fig. 16. Determination and correlation coefficients between accumulated rainfall and runoff for the 31-year period (1990 to 2020) in the studied soil.

Another important fact is that, due to low total porosity, hardsetting soils usually have low hydraulic conductivity (Lima Neto et al. 2009). The hydraulic conductivity (*Ks*) values directly affect the runoff results, since, depending on the *Ks* values, in high precipitation events, greater water losses via runoff will be simulated. The soil studied here had values of *Ks* equal to 15.0, 7.2, and 3.0 cm d<sup>-1</sup> for the 0-15, 15-30, and 30-45 cm depths, respectively. Especially in the deeper layers, the values are small, thus contributing to the fact that, during high-intensity precipitation events, part of the water will convert to runoff.

Differences were observed between WBCs obtained with deterministic values versus stochastic medians. We therefore confirm that deterministic modelling may generate results that do not correctly represent the parameters together with their uncertainties and correlations.

### 3.4. Conclusions

We tested the application of a previously developed stochastic technique to merge van Genuchten-Mualem parameters and associated statistics to stochastically predict water balance components using a 31-year historical data series. From the results we conclude that:

- i) Water balance components simulated deterministically using the mean hydraulic parameter values may be different from corresponding median values obtained from stochastic realizations. In our simulations, this was especially the case for bottom flux and transpiration. This shows the importance of stochastic analysis of uncertainty in vadose zone hydrological modelling;
- Some generated VGM parameters sets, as well as the accumulated rainfall and distribution during the crop cycle, are determining factors for the amplitude of variation of the simulated water balance components;
- iii) Except for transpiration data, the other water balance components (bottom flux, evaporation, and runoff) showed a clear correlation with the accumulated precipitation; In addition, the rainfall distribution throughout the crop cycle was decisive for results such as runoff. In high rainfall years, when less drought stress occurred, a significant reduction of stochastic variation in the simulated transpiration rate was noted.

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### 4. FINAL CONSIDERATIONS

The proposed stochastic method well represented the variability of the merged samples, mainly concerning the outputs of the water balance components generated by the model. Based on this and everything discussed in the two chapters presented in this work, we conclude that:

- The frequency distribution of predicted water balance components (bottom flux, evaporation, transpiration, and runoff) were very similar using the merged or the individual parameters;
- ii) Applying the technique to the period of 31 years, some generated VGM parameters sets, as well as the rainfall accumulation and distribution during the crop cycle, were determining factors to increase the dispersion of the water balance components results;
- iii) Except for transpiration data, the other water balance components (bottom flux, evaporation, and runoff) showed a good correlation with the accumulated precipitation;
- iv) The model predicted a significant reduction in the transpiration rate, especially in years with high precipitation;
- v) In general, using the mean hydraulic property parameter values to deterministically predict water balance components may yield values that are substantially different from the median values of stochastic realizations. This suggests that these values may generate unrepresentative results in hydrological modelling.

### **APPENDICES**

# Appendix A.

```
* Filename: ArthurTest.swp
* Contents: Main input data
* Comment area:
* Case: Chapadinha
*** GENERAL SECTION ***
*************************************
* Part 1: Environment
 PROJECT = 'Chapadinha'
                             ! Project description, [A80]
 PATHWORK = ' '
                                 ! Path to work folder, [A80]
 PATHATM = ' '
                         ! Path to folder with weather files, [A80]
                         ! Path to folder with crop files, [A80]
! Path to folder with drainage files, [A80]
 PATHCROP = ' '
 PATHDRAIN = ' '
 SWSCRE = 0
                          ! Switch, display progression of simulation run:
                             SWSCRE = 0: no display to screen
SWSCRE = 1: display water balance to screen
                          ! SWSCRE = 2: display daynumber to screen
                           ! Switch for printing errors to screen [Y=1, N=0]
***********************************
* Part 2: Simulation period
 TSTART = 01-jan-1990 ! Start date of simulation run, give day-month-year, [dd-mmm-yyyy]
        = 31-dec-2020 ! End date of simulation run, give day-month-year, [dd-mmm-yyyy]
***********************
* Part 3: Output dates
* Number of output times during a day
 NPRINTDAY = 1
                   ! Number of output times during a day, [1..1000, I]
* If NPRINTDAY = 1, specify dates for output of state variables and fluxes
                    ! Switch, output each month, [Y=1, N=0]
* If SWMONTH = 0, choose output interval and/or specific dates
                    ! Fixed output interval, ignore = 0, [0..366, I]
 SWRES = 0
                    ! Switch, reset output interval counter each year, [Y=1, N=0]
 SWODAT = 0
                    ! Switch, extra output dates are given in table, [Y=1, N=0]
* If SWODAT = 1, list specific dates [dd-mmm-yyyy], maximum MAOUT dates:
 OUTDATINT =
 31-Dec-2006
* End of table
* Output times for overall water and solute balances in *.BAL and *.BLC file
* Output can be provided at a fixed date in a year or at different dates:
 SWYRVAR = 0
                    ! SWYRVAR = 0: each year output of balances at the same date
                    ! SWYRVAR = 1: output of balances at different dates
* If SWYRVAR = 0 specify fixed date:
                   ! Specify day and month for output of yearly balances, [dd mm]
 DATEFIX = 31 12
* If SWYRVAR = 1 specify all output dates [dd-mmm-yyyy], maximum MAOUT dates:
 OIITD\DeltaT =
 31-dec-2006
* End of table
*************************
* Part 4: Output files
* General information
 OUTFIL = 'Result' ! Generic file name of output files, [A16]
```

```
SWHEADER = 0
                    ! Print header at the start of each balance period, [Y=1, N=0]
* Optional files
  SWVAP = 0
                   ! Switch, output profiles of moisture, solute and temperature, [Y=1, N=0]
  SWBLC = 1
                   ! Switch, output file with detailed yearly water balance, [Y=1, N=0]
  SWATE = 0
                   ! Switch, output file with soil temperature profiles, [Y=1, N=0]
  SWBMA = 0
                   ! Switch, output file with water fluxes, only for macropore flow, [Y=1, N=0]
  SWDRF = 0
                   ! Switch, output of drainage fluxes, only for extended drainage, [Y=1, N=0]
                   ! Switch, output surface water reservoir, only for extended drainage, [Y=1, N=0]
  SWSWB = 0
* Output for water quality models (PEARL, ANIMO) or other specific use (SWAFO to DZNEW)
* Optional output files
  SWAFO = 0
                   ! Switch, output file with formatted hydrological data
                   ! SWAFO = 0: no output
                   ! SWAFO = 1: output to a file named *.AFO
                   ! SWAFO = 2: output to a file named *.BFO
  SWAUN = 0
                   ! Switch, output file with unformatted hydrological data
                   ! SWAUN = 0: no output
                   ! SWAUN = 1: output to a file named *.AUN
                   ! SWAUN = 2: output to a file named *.BUN
* Critical deviation of water balance; in case of larger deviation, an error file is created
(*.DWB.CSV)
  CRITDEVMASBAL = 0.00001 ! Critical Deviation in water balance during PERIOD [0.0..1.0 cm, R]
st If SWAFO = 1 or 2, or SWAUN = 1 or 2: fine vertical discretization can be lumped
  SWDISCRVERT = 0 ! SWDISCRVERT = 0: no conversion
                   ! SWDISCRVERT = 1: convert vertical discretization,
* If SWDISCRVERT = 1 then specify:
  NUMNODNEW = 6 ! New number of nodes [1..macp, I, -]
 List thickness of each compartment, total thickness should correspond to Soil Water Section, part 4
           = 10.0 10.0 10.0 20.0 30.0 50.0 ! thickness of compartments [1.0d-6...5.0d2, cm, R]
*** METEOROLOGY SECTION ***
******************************
* General data
* File name
 METFIL = 'Chapadinha' ! File name of meteorological data without extension .YYY, [A200]
                       ! Extension is equal to last 3 digits of year, e.g. 003 denotes year 2003
* Use of reference evapotranspiration data from meteorological file instead of basic data
                       ! Switch, use reference ET values of meteo file [Y=1, N=0]
* If SWETR = 0, specify:
                        ! Latitude of meteo station, [-60..60 degrees, R, North = +]
 LAT = -3.40
 ALT = 37.
ALTW = 2.0
                       ! Altitude of meteo station, [-400..3000 m, R]
                         ! Altitude of wind speed measurement (10 m is default) [0..99 m, R]
  ANGSTROMA = 0.3136
                       ! Fraction of extraterrestrial radiation reaching the earth on overcast days
[0..1 -, R]
  ANGSTROMB = 0.3780
                           ! Additional fraction of extraterrestrial radiation reaching the earth on
clear days [0..1 -, R]
  SWDIVIDE =
                         ! 0 = Distribution E and T based on crop and soil factors
                         ! 1 = Distribution E and T based on direct application of Penman-Monteith
* Time interval of evapotranspiration and rainfall weather data
  SWMETDETAIL = 0
                       ! 0 = time interval is equal to one day
                       ! 1 = time interval is less than one day
* In case of detailed meteorological weather records (SWMETDETAIL = 1), specify:
                      ! Number of weather data records per day, [1..96 -, I]
  NMETDETAIL = 10
* In case of daily meteorological weather records (SWMETDETAIL = 0):
 SWETSINE = 0
                      ! Switch, distribute daily Tp and Ep according to sinus wave [Y=1, N=0]
  SWRAIN = 1
                       ! Switch for use of actual rainfall intensity (only if SWMETDETAIL = 0):
                       ! SWRAIN = 0: Use daily rainfall amounts
                       ! SWRAIN = 1: Use daily rainfall amounts + mean intensity
                       ! SWRAIN = 2: Use daily rainfall amounts + duration
```

```
! SWRAIN = 3: Use short time rainfall intensities, as supplied in separate file
* If SWRAIN = 1, then specify mean rainfall intensity RAINFLUX [0.d0..1000.d0 \, mm/d, \, R]
* as function of time TIME [0..366 d, R], maximum 30 records
   TIME
           RAINFLUX
   1.0
              500.0
 360.0
              500.0
* End of table
* If SWRAIN = 3, then specify file name of file with detailed rainfall data
 RAINFIL = 'WagRain'
                        ! File name of detailed rainfall data without extension .YYY, [A200]
                        ! Extension is equal to last 3 digits of year, e.g. 003 denotes year 2003
*** CROP SECTION ***
***********************************
* Part 1: Crop rotation scheme
* Switch for bare soil or cultivated soil
 SWCROP = 1 ! 0 = Bare soil
             ! 1 = Cultivated soil
* Specify for each crop (maximum MACROP):
* INITCRP
             = type of initialisation of crop growth: emergence (default) = 1, sowing = 2 [-]
* CROPSTART = date of crop emergence, [dd-mmm-yyyy]
* CROPEND
             = date of crop harvest, [dd-mmm-yyyy]
* CROPNAME
             = crop name, [A16]
 CROPFIL
            = name of file with crop input parameters without extension .CRP, [A16]
* CROPTYPE
           = type of crop model: simple = 1, detailed general = 2, detailed grass = 3
 CROPSTART
                 CROPEND
                                CROPNAME
                                          CROPFIL
                                                       CROPTYPE
                                         'SoyBeanD'
                                'Soy'
                 01-jun-1990
 01-feb-1990
                                                         2
 15-jun-1990
                 30-sep-1990
                                'Gmaize
                                         'GmaizeD'
                                                         2
 01-feb-1991
                 01-jun-1991
                                'Soy'
                                         'SoyBeanD'
                                                         2
 15-jun-1991
                                'Gmaize'
                                         'GmaizeD'
                 30-sep-1991
                                                         2
 01-feb-1992
                 01-jun-1992
                                'Soy'
                                         'SoyBeanD'
                                                         2
 15-jun-1992
                 30-sep-1992
                                'Gmaize'
                                         'GmaizeD'
                                                         2
                                'Soy'
                                         'SoyBeanD'
 01-feb-1993
                 01-jun-1993
                                                         2
 15-jun-1993
                 30-sep-1993
                                'Gmaize'
                                         'GmaizeD'
                                                         2
 01-feb-1994
                 01-jun-1994
                                'Soy'
                                         'SoyBeanD'
                                                         2
 15-jun-1994
                                'Gmaize'
                                         'GmaizeD'
                 30-sep-1994
                                                         2
                                'Soy'
                                         'SoyBeanD'
 01-feb-1995
                 01-jun-1995
                                                         2
 15-jun-1995
                 30-sep-1995
                                'Gmaize'
                                         'GmaizeD'
                                                         2
                                'Soy'
                                         'SoyBeanD'
                 01-jun-1996
 01-feb-1996
                                                         2
 15-jun-1996
                 30-sep-1996
                                'Gmaize'
                                         'GmaizeD'
                                                         2
 01-feb-1997
                 01-jun-1997
                                'Soy'
                                         'SoyBeanD'
                                                         2
                                'Gmaize'
                                         'GmaizeD'
 15-jun-1997
                 30-sep-1997
                                                         2
  01-feb-1998
                 01-jun-1998
                                'Soy'
                                         'SoyBeanD'
                                                         2
 15-jun-1998
                 30-sep-1998
                                'Gmaize'
                                         'GmaizeD'
                                                         2
                                'Soy'
                                          'SoyBeanD'
 01-feb-1999
                 01-jun-1999
                                                         2
                                'Gmaize'
                                         'GmaizeD'
                                                         2
 15-jun-1999
                 30-sep-1999
 01-feb-2000
                 01-jun-2000
                                'Soy'
                                          'SoyBeanD'
                                                         2
                                'Gmaize'
                                         'GmaizeD'
 15-jun-2000
                 30-sep-2000
                                                         2
  01-feb-2001
                 01-jun-2001
                                'Soy'
                                                         2
                                         'SoyBeanD'
 15-jun-2001
                 30-sep-2001
                                'Gmaize'
                                         'GmaizeD'
                                                         2
                                'Soy'
                                          'SoyBeanD'
 01-feb-2002
                 01-jun-2002
                                                         2
                                'Gmaize'
                                         'GmaizeD'
 15-jun-2002
                 30-sep-2002
                                                         2
 01-feb-2003
                                'Soy'
                                          'SoyBeanD'
                 01-jun-2003
                                                         2
                                'Gmaize'
 15-jun-2003
                 30-sep-2003
                                         'GmaizeD'
                                                         2
  01-feb-2004
                                'Soy'
                                                          2
                 01-jun-2004
                                         'SoyBeanD'
 15-jun-2004
                 30-sep-2004
                                'Gmaize'
                                         'GmaizeD'
                                                         2
                                'Soy'
 01-feb-2005
                 01-jun-2005
                                          'SoyBeanD'
                                                         2
 15-jun-2005
                 30-sep-2005
                                'Gmaize'
                                         'GmaizeD'
                 01-jun-2006
                                'Soy'
 01-feb-2006
                                          'SovBeanD'
                                                         2
 15-jun-2006
                 30-sep-2006
                                'Gmaize'
                                         'GmaizeD'
                                                         2
 01-feb-2007
                 01-jun-2007
                                'Soy'
                                         'SoyBeanD'
                                                         2
 15-iun-2007
                                'Gmaize'
                                         'GmaizeD'
                                                         2
                 30-sen-2007
                                'Soy'
 01-feb-2008
                 01-jun-2008
                                          'SoyBeanD'
                                                         2
 15-jun-2008
                 30-sep-2008
                                'Gmaize
                                         'GmaizeD'
                                'Soy'
                                         'SoyBeanD'
 01-feb-2009
                 01-jun-2009
                                                         2
```

15-jun-2009

01-feb-2010

15-jun-2010

01-feb-2011

30-sep-2009

01-jun-2010

30-sep-2010

01-jun-2011

'Gmaize'

'Gmaize'

'Soy'

'Soy'

'GmaizeD'

'SoyBeanD'

'GmaizeD'

'SoyBeanD'

2

2

2

2

```
15-jun-2011
                 30-sep-2011
                               'Gmaize'
                                        'GmaizeD'
                 01-jun-2012
  01-feb-2012
                               'Soy'
                                        'SoyBeanD'
                               'Gmaize
                                        'GmaizeD'
  15-jun-2012
                 30-sep-2012
  01-feb-2013
                 01-jun-2013
                                        'SoyBeanD'
                               'Soy'
  15-jun-2013
                 30-sep-2013
                               'Gmaize
                                        'GmaizeD'
                               'Soy'
                                        'SoyBeanD'
  01-feb-2014
                 01-jun-2014
  15-jun-2014
                 30-sep-2014
                               'Gmaize'
                                       'GmaizeD'
  01-feb-2015
                               'Soy'
                 01-jun-2015
                                        'SoyBeanD'
                               'Gmaize
                                       'GmaizeD'
  15-jun-2015
                 30-sep-2015
  01-feb-2016
                 01-jun-2016
                               'Soy'
                                        'SoyBeanD'
                 30-sep-2016
  15-iun-2016
                               'Gmaize' 'GmaizeD'
                               'Soy'
                                        'SoyBeanD'
  01-feb-2017
                 01-jun-2017
  15-jun-2017
                 30-sep-2017
                               'Gmaize'
                                       'GmaizeD'
                               'Soy'
                 01-jun-2018
                                        'SoyBeanD'
  01-feb-2018
                               'Gmaize
                                       'GmaizeD'
  15-jun-2018
                 30-sep-2018
                                                        2
  01-feb-2019
                 01-jun-2019
                               'Soy'
                                        'SoyBeanD'
                 30-sep-2019
  15-jun-2019
                               'Gmaize'
                                       'GmaizeD'
                                                        2
  01-feb-2020
                 01-jun-2020
                               'Soy'
                                        'SoyBeanD'
                                                        2
  15-jun-2020
                 30-sep-2020
                               'Gmaize'
                                       'GmaizeD'
* End of table
************************************
**********************************
* Part 2: Fixed irrigation applications
* Switch for fixed irrigation applications
  SWIRFIX = 0
                ! SWIRFIX = 0: no irrigation applications are prescribed
                 ! SWIRFIX = 1: irrigation applications are prescribed
* If SWIRFIX = 1, specify:
* Switch for separate file with fixed irrigation applications
  SWIRGFIL = 0 ! SWIRGFIL = 0: data are specified in the .swp file
                 ! SWIRGFIL = 1: data are specified in a separate file
* If SWIRGFIL = 0 specify information for each fixed irrigation event (max. MAIRG):
* IRDATE = date of irrigation, [dd-mmm-yyyy]
* IRDEPTH = amount of water, [0.0..100.0 cm, R]

* IRCONC = concentration of irrigation water, [0.0..1000.0 mg/cm3, R]

* IRTYPE = type of irrigation: sprinkling = 0, surface = 1
       IRDATE
               IRDEPTH
                            IRCONC
                                    IRTYPE
  05-jan-1994
                            1000.0
                   0.5
* end of table
* If SWIRGFIL = 1, specify name of file with data of fixed irrigation applications:
  IRGFIL = 'testirri'
                          ! File name without extension .IRG [A16]
*** SOIL WATER SECTION ***
*************************
* Part 1: Initial soil moisture condition
 SWINCO = 1 ! Switch, type of initial soil moisture condition:
            ! 1 = pressure head as function of depth is input
            ! 2 = pressure head of each compartment is in hydrostatic equilibrium
                  with initial groundwater level
            ! 3 = read final pressure heads from output of previous Swap simulation
* If SWINCO = 1, specify (maximum MACP):
* ZI = soil depth, [-10000..0 cm, R]
* H = initial soil water pressure head, [-1.d10..1.d4 cm, R]
     ΖI
             -15.0
     0.0
  -100.0
            -15.0
* End of table
* If SWINCO = 2, specify:
  GWLI = -75.0 ! Initial groundwater level, [-10000..100 cm, R]
* If SWINCO = 3, specify:
  INIFIL = 'result.end' ! name of final with extension .END [a200]
```

```
************************************
* Part 2: Ponding, runoff and runon
* Ponding
 PONDMX = 0.2 ! In case of ponding, minimum thickness for runoff, [0..1000 cm, R]
         = 0.5 ! Drainage resistance for surface runoff [0.001..1.0 d, R]
 RSROEXP = 1.0 ! Exponent in drainage equation of surface runoff [0.1..10.0 -, R]
* Runon
* Specify whether runon data are provided in extra input file
  SWRUNON = 0 ! 0 = No input of runon data
              ! 1 = Runon data are provided in extra input file
* If SWRUNON = 1, specify name of file with runon input data
* This file may be an output *.inc file (with only 1 header) of a previous Swap-simulation
 RUFIL = 'runon.inc' ! File name with extension [A80]
*************************************
************************************
* Part 3: Soil evaporation
 CFEVAPPOND = 1.25 ! When ETref is used, evaporation coefficient in case of ponding [0..3 -, R]
            ! Switch for use of soil factor CFBS to calculate Epot from ETref
 SWCFBS = 0
              ! 0 = soil factor is not used
              ! 1 = soil factor is used
* If SWCFBS = 1, specify soil factor CFBS:
 CFBS = 0.5 ! Soil factor CFBC in Epot = CFBS * ETref [0..1.5 -, R]
* If SWDIVIDE = 1 (partitoning according to PMdirect) specify minimum soil resistance
 RSOIL = 150.0 ! Soil resistance of wet soil [0..1000.0 s/m, R]
 SWRFDU = 1
             ! Switch, method for reduction of potential soil evaporation:
              ! 0 = reduction to maximum Darcy flux
              ! 1 = reduction to maximum Darcy flux and to maximum Black (1969)
              ! 2 = reduction to maximum Darcy flux and to maximum Boesten/Stroosnijder (1986)
 COFRED = 0.35 ! Soil evaporation coefficient of Black [0..1 cm/d1/2, R],
              ! or Boesten/Stroosnijder [0..1 cm1/2, R]
RSIGNI = 0.5 ! Minimum rainfall to reset method of Black [0..1 cm/d, R]
* Part 4: Vertical discretization of soil profile
* Specify the following data (maximum MACP lines):
* ISOILLAY = number of soil layer, start with 1 at soil surface, [1..MAHO, I]
* ISUBLAY = number of sub layer, start with 1 at soil surface, [1..MACP, I] 
* HSUBLAY = height of sub layer, [0.0..1000.0 cm, R]
* HCOMP
        = height of compartments in this layer, [0.0..1000.0 cm, R]
         = number of compartments in this layer (= HSUBLAY/HCOMP), [1..MACP, I]
 ISOILLAY ISUBLAY HSUBLAY
                            HCOMP
                                     NCOMP
          1
                 15.0
                            1.0
                                     15
    1
    2
            2
                   15.0
                             1.0
                                      15
                   45.0
                             1.0
* end of table
*******************************
* Part 5: Soil hydraulic functions
* Specify for each soil layer (maximum MAHO):
* ISOILLAY1 = number of soil layer, as defined in part 4 [1..MAHO, I]
* ORES = Residual water content, [0..0.4 cm3/cm3, R]
* OSAT
        = Saturated water content, [0..0.95 cm3/cm3, R]
       = Shape parameter alfa of main drying curve, [0.0001..1 /cm, R]
* ALFA
```

```
* NPAR
       = Shape parameter n, [1..4 -, R]
       = Saturated vertical hydraulic conductivity, [1.d-5..1000 cm/d, R]
* KSAT
* LEXP
       = Exponent in hydraulic conductivity function, [-25..25 -, R]
* ALFAW = Alfa parameter of main wetting curve in case of hysteresis, [0.0001..1 /cm, R]
* H_ENPR = Air entry pressure head [-40.0..0.0 cm, R]
 ISOILLAY1 ORES
                 OSAT
                       ALFA
                               NPAR
                                               LEXP
                                                       ALFAW H_ENPR
                0.3374 0.0792 2.4809 15.0000
                                                      0.5000 0.0792
      1 0.0000
                                                                       0.0000
                                                      0.5000
                                                               0.1018 0.0000
         0.0000 0.3001 0.1018 2.5206
                                           15.0000
                 0.2753 0.0535 2.8546
                                           15.0000
                                                      0.5000
                                                              0.0535 0.0000
      3
         0.0000
* --- end of table
************************************
*************************
* Part 6: Hysteresis of soil water retention function
* Switch for hysteresis:
 SWHYST = 0
             ! 0 = no hysteresis
             ! 1 = hysteresis, initial condition wetting
             ! 2 = hysteresis, initial condition drying
* If SWHYST = 1 or 2, specify:
 TAU = 0.2 ! Minimum pressure head difference to change wetting-drying, [0..1 cm, R]
*************************
* Part 7: Maximum rooting depth
 RDS = 75.0 ! Maximum rooting depth allowed by the soil profile, [1..5000 cm, R]
********************************
* Part 8: Similar media scaling of soil hydraulic functions
 SWSCAL = 0 ! Switch for similar media scaling [Y=1, N=0]; no hysteresis is allowed
           ! in case of similar media scaling (SWHYST = 0)
* If SWSCAL = 1, specify:
 NSCALE = 3 ! Number of simulation runs, [1..MASCALE, I]
* Supply the scaling factors for each simulation run and each soil layer:
 RUN
        SOIL1
                    SOIL2
         0.5
  1
                    2.0
  2
         1.0
                     1.0
  3
         2.0
                     0.5
  4
         1.0
                     1.0
  5
         3.0
                     3.0
* End of table
* Part 9: Preferential flow due to macropores
 SWMACRO = 0
                ! Switch for macropore flow, [0..2, I]:
               ! 0 = no macropore flow
               ! 1 = macropore flow
***********************************
* Part 10: Snow and frost
* Snow
 SWSNOW = 0 ! Switch, calculate snow accumulation and melt, [Y=1, N=0]
* If SWSNOW = 1, specify:
 SNOWINCO = 22.0
                    ! Initial snow water equivalent, [0.0...1000.0 cm, R]
 TEPRRAIN = 2.0
                    ! Temperature above which all precipitation is rain, [ 0.0...5.0 °C, R]
                 ! Temperature below which all precipitation is snow,[-5.0...0.0 ºC, R]
! Snowmelt calibration factor, [0.0...10.0 -, R]
 TEPRSNOW = -2.0
 SNOWCOEF = 0.3
* Frost
 SWFROST = 0 ! Switch, in case of frost: reduce soil water flow, [Y=1, N=0]
```

```
* If SWFROST = 1, then specify soil temperature to start end end flux-reduction
                    ! Soil temperature (ºC) where reduction of water fluxes starts [-10.0,5.0, oC,
 tfroststa = 0.0
R]
                  ! Soil temperature (°C) where reduction of water fluxes ends [-10.0,5.0, oC, R]
 tfrostend = -1.0
*************************************
***********************************
* Part 11 Numerical solution of Richards' equation
 DTMIN
               = 1.0d-4
                           ! Minimum timestep, [1.d-7..0.01 d, R]
                         ! Maximum timestep, [ 0.01..0.5 d, R]
 DTMAX
              = 0.2
              = 100.0
 GWLCONV = 100.0 ! Maximum dif. groundwater level between iterations, [1.d-5..1000 cm, R] CritDevPondDt = 1.0d-4 ! Maximum water balance error of ponding layer, [1.0d-6..0.1 cm, R]
          = 30 ! Maximum number of iteration cycles, [5..100 -, I]
= 3 ! Maximum number of back track cycles within an iteration cycle, [1..10 -
 MaxIt
 MaxBackTr
,I]
* Switch for mean of hydraulic conductivity, [1..4 -, I]:
* 1 = unweighted arithmic mean; 2 = weighted arithmic mean
* 3 = unweighted geometric mean; 4 = weighted geometric mean
 SWkmean = 1
* Switch for explicit/implicit solution Richards equation with hydraulic conductivity, [1..2 -, I]:
 SWkImpl = 0 ! 0 = explicit solution
              ! 1 = implicit solution
************************
*** LATERAL DRAINAGE SECTION ***
************************************
* Specify whether lateral drainage to surface water should be included
 SWDRA = 0 ! Switch, simulation of lateral drainage:
            ! 0 = No simulation of drainage
            ! 1 = Simulation with basic drainage routine
            ! 2 = Simulation of drainage with surface water management
* If SWDRA = 1 or SWDRA = 2 specify name of file with drainage input data:
 DRFIL = 'Hupsel' ! File name with drainage input data without extension .DRA, [A16]
*** BOTTOM BOUNDARY SECTION ***
************************************
* Bottom boundary condition
                  ! Switch for file with bottom boundary conditions:
 SWBBCFILE = 0
                  ! SWBBCFILE = 0: data are specified in the .swp file
                  ! SWBBCFILE = 1: data are specified in a separate file
* If SWBBCFILE = 1 specify name of file with bottom boundary conditions:
                  ! File name without extension .BBC [A16]
 BBCFIL = ' '
* If SWBBCFILE = 0, select one of the following options:
            ! 1 Prescribe groundwater level
            ! 2 Prescribe bottom flux
            ! 3 Calculate bottom flux from hydraulic head of deep aquifer
            ! 4 Calculate bottom flux as function of groundwater level
            ! 5 Prescribe soil water pressure head of bottom compartment
! 6 Bottom flux equals zero
            ! 7 Free drainage of soil profile
            ! 8 Free outflow at soil-air interface
SWBOTB = 7 ! Switch for bottom boundary [1..8,-,I]
* Options 6,7 and 8 require no additional bottom input data
************************************
```

\* End of the main input file .SWP! @

## Appendix B.

```
* Filename: SoyBeanD.crp
* Contents: SWAP 3.2 - Data for detailed crop model
************************************
* Soybean (Glycine max (L.) Merrill)
*** PLANT GROWTH SECTION ***
*************************************
* Part 1: Crop factor or crop height
 SWCF = 2 ! choice between crop factor [=1] or crop height [=2]
* Choose crop factor if ETref is used, either from meteo input file (SWETR = 1) or with Penman-Monteith
* Choose crop height if Penman-Monteith should be used with actual crop height, albedo and resistance
* If SWCF = 1, list crop factor CF [0.5..1.5, R], as function of dev. stage DVS [0..2 -, R]: * If SWCF = 2, list crop height CH [0..1000 \text{ cm}, R], as function of dev. stage DVS [0..2 -, R]:
* (maximum 36 records)
   DVS
           CH
                 CF
   0.0
          25.0
                1.0
   1.0
          60.0
                 1.2
   2.0
          80.0
                 1.2
* End of Table
* If SWCF = 2, list crop specifi values for:
 ALBEDO = 0.23 ! crop reflection coefficient [0..1.0 -, R]
 RSC
      = 70.0 ! Minimum canopy resistance [0..10^6 s/m, R]
           0.0 ! Canopy resistance of intercepted water [0..10^6 s/m, R]
* Part 2 : Crop development
 IDSL =
               0 ! Switch:
                  0 = Crop development before anthesis depends on temperature only
                  1 = Crop development before anthesis depends on daylength only
                  2 = Crop development before anthesis depends on both
* If IDSL = 1 or 2, specify:
      = 14.0
                 ! Optimum daylength for crop development [0..24 h, R]
 DLC
       = 8.0
                 ! Minimum daylength, [0..24 h, R]
* If IDSL = 0 or 2 specify:
 TSUMEA = 1150.00 ! Temperature sum from emergence to anthesis, [0..10000 C, R]
 TSUMAM = 950.00 ! Temperature sum from anthesis to maturity [0..10000 C, R]
* List increase in temperature sum [0..60 C, R] as function of daily average temp. [0..100 C, R]
        TAV DTSM
                   (maximum 15 records)
 DTSMTB =
          0.00
               0.00
         10.00
               0.00
         20.00 10.00
         35.00 25.00
         60.00 25.00
* End of Table
            2.00 ! development stage at harvest [-]
* Part 3: Initial values
 TDWI
      = 120.000 ! Initial total crop dry weight [0..10000 kg/ha, R]
 LAIEM = 0.0163 ! Leaf area index at emergence [0..10 m2/m2, R]
 RGRLAI = 0.00500 ! Maximum relative increase in LAI [0..1 m2/m2/d, R]
* Part 4: Green surface area
* List specific leaf area [0..1 \text{ ha/kg, R}] as function of devel. stage [0..2, R]
```

```
DVS SLA
                  (maximum 15 records)
 SLATB =
         0.00 0.0014
         0.45 0.0025
         0.90 0.0025
         2.00 0.0007
* End of Table
 SPA
       = 0.0000 ! Specific pod area [0..1 ha/kg, R]
          0.0000 ! Specific stem area [0..1 ha/kg, R]
 SSA
         23.00 ! Life span under leaves under optimum conditions, [0..366 d, R]
 SPAN
          15.00 ! Lower threshold temperature for ageing of leaves ,[-10..30 C, R]
          ******************
******************************
* Part 5: Assimilation
 KDIF
            0.50! Extinction coefficient for diffuse visible light, [0..2 -, R] !.50
 KDIR
            0.75 ! Extinction coefficient for direct visible light, [0..2 -, R] !.75
            0.40 ! Light use efficiency for real leaf [0..10 kg/ha/hr/(Jm2s), R] !.40
 EFF
 List max CO2 assimilation rate [0..100 kg/ha/hr, R] as function of development stage [0..2 -, R]
                    (maximum 15 records)
         DVS
               AMAX
 AMAXTB =
         0.00 37.000
         1.60 37.000
         2.00 0.000
* End of table
st List reduction factor of AMAX [-, R] as function of average day temp. [-10..50 C, R]
         TAVD
              TMPF (maximum 15 records)
 TMPFTB =
         0.00 0.000
        10.00
              0.300
        20.00 0.600
        25.00
              0.800
        30.00
              1.000
        35.00
              1.000
* End of table
 List reduction factor of AMAX [-, R] as function of minimum day temp. [-10..50 C, R]
              TMNF (maximum 15 records)
 TMNFTB =
         0.00 0.000
         3.00 1.000
* End of table
* Part 6: Conversion of assimilates into biomass
       = 0.6800 ! Efficiency of conversion into leaves,
                                                         [0..1 \text{ kg/kg, R}]
       = 0.7200 ! Efficiency of conversion into storage organs, [0..1 kg/kg, R]
 CVO
       = 0.7200 ! Efficiency of conversion into roots,
 CVR
                                                         [0..1 \text{ kg/kg, R}]
       = 0.6900 ! Efficiency of conversion into stems,
 CVS
                                                         [0..1 \text{ kg/kg, R}]
* Part 7: Maintenance respiration
 010
          2.0000 ! Rel. increase in respiration rate with temperature, [0..5 /10 C, R]
          0.0300 ! Rel. maintenance respiration rate of leaves, [0..1 kgCH2O/kg/d, R]
       = 0.0100 ! Rel. maintenance respiration rate of st. org.,[0..1 kgCH2O/kg/d, R]
 RMO
 RMR
          0.0100 ! Rel. maintenance respiration rate of roots,
                                                         [0..1 kgCH2O/kg/d, R]
       = 0.0150 ! Rel. maintenance respiration rate of stems,
                                                         [0..1 kgCH2O/kg/d, R]
^{st} List reduction factor of senescence [-, R] as function of dev. stage [0..2 -, R]
               RFSE (maximum 15 records)
 RFSETB =
         0.00
               1.00
         2.00
               1.00
* End of table
* Part 8: Partitioning
```

```
* List fraction of total dry matter increase partitioned to the roots [kg/kg, R]
* as function of development stage [0..2 -, R]
           DVS
                   FR
                         (maximum 15 records)
  FRTB =
           0.00
                  0.50
           0.75
                  0.10
           1.50
                  0.00
           2.00
                  0.00
* End of table
* List fraction of total above ground dry matter incr. part. to the leaves [kg/kg, R]
st as function of development stage [0..2 -, R]
           DVS
                   FL
                        (maximum 15 records)
  FLTB =
           0.00
                  0.75
           1.00
                  0.75
                  0.60
           1.15
           1.30
                  0.46
           1.50
                  0.27
           1.70
                  0.00
           2.00
                  0.00
* End of table
^{*} List fraction of total above ground dry matter incr. part. to the stems [kg/kg, R]
 as function of development stage [0..2 -, R]
           DVS
                  FS (maximum 15 records)
 FSTB =
           0.00
                  0.25
           1.00
                  0.25
           1.15
                  0.27
           1.30
                  0.27
           1.50
                  0.28
           1.70
                  0.00
           2.00
                  0.00
* End of table
* List fraction of total above ground dry matter incr. part. to the st. organs [kg/kg, R]
* as function of development stage [0..2 -, R]
           DVS
                  FO
                        (maximum 15 records)
  FOTB =
           0.00
                  0.00
           1.00
                  0.00
           1.15
                  0.13
           1.30
                  0.27
           1.50
                  0.45
           1.70
                  1.00
           2.00
                  1.00
* End of table
* Part 9: Death rates
  PFRDI =
           0.030 ! Maximum rel. death rate of leaves due to water stress [0..3 /d, R]
* List relative death rates of roots [kg/kg/d] as function of dev. stage [0..2 -, R]
           DVS
                  RDRR
                          (maximum 15 records)
  RDRRTB =
          0.0000 0.0000
          1.5000 0.0000
          1.5001 0.0200
          2.0000 0.0200
* End of table
* List relative death rates of stems [kg/kg/d] as function of dev. stage [0..2 -, R]
           DVS
                   RDRS
                           (maximum 15 records)
  RDRSTB =
          0.0000 0.0000
          1.5000 0.0000
          1.5001 0.0200
          2,0000 0,0200
* End of table
```

\* Part 10: Crop water use

```
! Switch for type root water extraction [1,2 -, I]
 swroottyp = 1
                   ! (1 = Feddes et al., 1978; 2 = De Jong van Lier et al., 2006)
st if swroottyp=1 then enter HLIM1 - ADCRL
* if swroottyp=2 then enter wiltpoint, rootradius, rootcoefa
 HLIM1 =
             -2.0 ! No water extraction at higher pressure heads, [-100..100 cm, R]
             -5.0 ! h below which optimum water extr. starts for top layer, [-1000..100 cm, R]
 HLIM2U =
             -5.0! h below which optimum water extr. starts for sub layer, [-1000..100 cm, R]
 HLIM2L =
            -400.0 ! h below which water uptake red. starts at high Tpot, [-10000..100 cm, R] !-200 -500.0 ! h below which water uptake red. starts at low Tpot, [-10000..100 cm, R] !-350
 HLIM3H =
 HITM3I =
 HLIM4 =
           -5000.0 ! No water extraction at lower pressure heads, [-16000..100 cm, R]
 ADCRH =
               0.5 ! Level of high atmospheric demand, [0..5 cm/d, R]
               0.1 ! Level of low atmospheric demand, [0..5 cm/d, R]
 ADCRL =
* Part 11: salt stress
* only when solutes are simulated (SWSOLU=1 in SWP-file)
* relation between ECsat and crop reduction
               5.0 ! ECsat level at which salt stress starts, [0..20 dS/m, R]
 ECSLOP =
              20.0 ! Decline of rootwater uptake above ECMAX [0..40 %/dS/m, R]
* relation between concentration and ECsat
             4.21 ! coefficient a to convert concentration to EC [0.0..1000.0 -, R]
 C2ECa =
             0.763 ! exponent b to convert concentration to EC [0.0..10.0 -, R]
* Switch to enter factor f (SWC2ECF ) per profile or per soil layer/horizon [1,2 -, I]
    if SWC2ECF = 1 then enter one C2ECf-value for whole model profile
    if SWC2ECF = 2 then enter one C2ECf-value for each model/soil layer/horizon
 SWC2ECF = 1
* factor f to convert concentration to EC [0.0..10.0 -, R];
    dependent on SWC2ECF one value for model profile or a value for each soil horizon
 C2ECf = 1.7
**************************************
* Part 12: Interception
* For agricultural crops apply interception concept of Von Hoyningen-Hune and Braden
 SWINTER = 1 ! Switch for rainfall interception method:
               ! 0 = No interception calculated
               ! 1 = Agricultural crops (Von Hoyningen-Hune and Braden)
              ! 2 = Trees and forests (Gash)
 COFAR =
              0.25 ! Interception coefficient Von Hoyningen-Hune and Braden, [0..1 cm, R]
************************************
* Part 13: Root density distribution and root growth
* List relative root density [0..1 -, R], as function of rel. rooting depth [0..1 -, R]:
          RD
                RDC (maximum 11 records)
 RDCTB =
          0.00
                1.00
                1.00 !0.2 antes
          1.00
 End of table
 RDI
             5.00 ! Initial rooting depth, [0..1000 cm, R]
             1.20 ! Maximum daily increase in rooting depth, [0..100 cm/d, R]
            75.00 ! Maximum rooting depth crop/cultivar, [0..1000 cm, R] !antes 45.00
***********************************
*** IRRIGATION SCHEDULING SECTION ***
***********************************
* Part 1: General
 SCHEDULE = 0 ! Switch for application irrigation scheduling [Y=1, N=0]
* If SCHEDULE = 0, no more information is required in this input file!
* End of .crp file !
```

## Appendix C.

```
**************************************
* Filename: GMaizeD.CRP
* Contents: SWAP 3.2 - Data for detailed crop model
                             ******************
*c Grain maize (Zea mays L.)
** $Id: mag201.cab 1.3 1997/09/25 14:06:58 LEM release $
** File MAG201.CAB
** CROP DATA FILE for use with WOFOST Version 5.4, June 1992
** GRAIN MAIZE 201
** Regions : Germany, R13, R15, R16, R17 and Luxembourg
** sowing date 1 May
** mean date of flowering 26 July, mature 20 October
** Derived from SUCROS87 data set for maize.
** Calibrated for use in WOFOST model at the Centre for Agrobiological
** Research (CABO-DLO) for the simulation of crop growth and yield on the
** basis of daily weather data.
** Purpose of application: Crop growth monitoring with agrometeorological
** model in the EC.
** Developed in the framework of JRC Agriculture Project Action 3.
** Input Differences with WOFOST
* - Input part for additional parameters for ET-calculations (Part 1)
st - Germination also due to soil moisture conditions (HDRYGERM .. BGERM)
* - Input of Extinction coefficient for direct visible light (KDIR)
* - No input of water use params (CFET, DEPNR, IAIRDU); these are determined by Swap-modules
st - Input part for Soil water extraction by plant roots (Part 10)
* - Input part for salt stress (Part 11)
* - Input part for interception (Part 12)
* - Input of rooting depth (density) as function of depth (RDCTB) (Part 13)
* - Expert-option for rooting depth limitation by relative dry matter increase (Part 13:SWDMI2RD)
       Input part for stress
                                     due to management other than irrigation,
                                                                                          e.g.
pests, diseases, nutrients, etc.. (Part 14)
* - Seperate section for irrigation scheduling (Part 15,16,17)
*** PLANT GROWTH SECTION ***
**********************************
* Part 1: Crop factor or crop height
 SWCF = 2 ! choice between crop factor [=1] or crop height [=2]
* Choose crop factor if ETref is used, either from meteo input file (SWETR = 1) or with Penman-Monteith
* Choose crop height if Penman-Monteith should be used with actual crop height, albedo and resistance
* If SWCF = 1, list crop factor CF [0.5..1.5, R], as function of dev. stage DVS [0..2 -, R]: * If SWCF = 2, list crop height CH [0..1000 \text{ cm}, R], as function of dev. stage DVS [0..2 -, R]:
* (maximum 36 records)
        DVS
               CH CF
               1.0 0.5
        0.0
        0.3
              15.0 0.8
              40.0 1.0
        0.5
        0.7
            140.0 1.0
             170.0 1.0
        1.0
             180.0 1.0
        1.4
            175.0 1.0
        2.0
* End of Table
* If SWCF = 2, list crop specifi values for:
  ALBEDO = 0.20 ! crop reflection coefficient [0..1.0 -, R]
       = 131.0 ! Minimum canopy resistance [0..10^6 s/m, R]
            0.0 ! Canopy resistance of intercepted water [0..10^6 s/m, R]
**************************************
*********************************
* Part 2 : Crop development
 IDSL
                0 ! Switch for crop development:
                    0 = Crop development before anthesis depends on temperature only
                    1 = Crop development before anthesis depends on daylenght e only
                    2 = Crop development before anthesis depends on both
```

```
* If IDSL = 1 or 2, specify:
                    ! Minimum day length for optimum crop development [0..24 h, R]
 DLO = 1.0
                    ! Shortest day length for any development, [0..24 h, R]
* If IDSL = 0 or 2 specify:
 TSUMEA = 600.00 ! Temperature sum from emergence to anthesis, [0..10000 C, R]
  TSUMAM =
            750.00 ! Temperature sum from anthesis to maturity [0..10000 C, R]
st List increase in temperature sum [0..60 C, R] as function of daily average temp. [0..100 C, R]
                      (maximum 15 records)
         TAV DTSM
 DTSMTB =
                  0.00
           0.00
           6.00
                  0.00
           30.00 24.00
           35.00 24.00
* End of Table
 DVSEND =
                2.00 ! development stage at harvest [-]
* germination defined in .swp-file :
  INITCRP=1: CROPSTART defines emergence (default), INITCRP=2: CROPSTART defines sowing
 IF INITCRP = 2 specify
 TSUMEMEORT =
                 70.0 ! temperature sum needed for crop emergence
                                                                          [0..1000 C d, R]
 TBASEM
                  6.0 ! minimum temperature, used for germination trajectory [0..40 C, R]
             = 30.0 ! maximum temperature, used for germination trajectory [0..40 C, R]
= -500.0 ! pressure head rootzone for dry germination trajectory [-1000..-0.01 cm, R]
  TFFFMX
 HDRYGERM
 HWETGERM
             = -50.0 ! pressure head rootzone for wet germination trajectory [-100..-0.01 cm, R]
             = 203. ! a-coefficient Eq. 24/25 Feddes & Van Wijk
= -432. ! c-coefficient Eq. 24 Feddes & Van Wijk
 AGERM
                                                                          [1..1000, R]
                                                                          [1..1000, R]
 CGFRM
 BGERM
             = 522.
                        ! b-coefficient Eq. 25
                                                  Feddes & Van Wijk
                                                                          [1..1000, R]
*******************************
* Part 3: Initial values
 TDWI = 200.00
                    ! Initial total crop dry weight [0..10000 kg/ha, R] !20
 LAIEM = 0.04836
                    ! Leaf area index at emergence [0..10 m2/m2, R]
                   ! Maximum relative increase in LAI [0..1 m2/m2/d, R]
 RGRI \Delta T = 0.02940
* Part 4: Green surface area
         = 0.0000 ! Specific pod area [0..1 ha/kg, R]
           0.0000 ! Specific stem area [0..1 ha/kg, R]
             33.00 ! Life span under leaves under optimum conditions, [0..366 d, R] !33
 TBASE =
            10.00 ! Lower threshold temperature for ageing of leaves ,[-10..30 C, R] !4
* List specific leaf area [0..1 ha/kg, R] as function of devel. stage [0..2, R]
         DVS SLA
                      (maximum 15 records)
 SLATB =
           0.00 0.0026
           0.78 0.0012
           2.00 0.0012
* End of Table
* Part 5: Assimilation
 KDIF
              0.60 ! Extinction coefficient for diffuse visible light, [0..2 -, R]
 KDIR
              0.75 ! Extinction coefficient for direct visible light, [0..2 -, R]
             0.45 ! Light use efficiency for real leaf [0..10 kg CO2 /J adsorbed), R] \,
 EFF
 List max CO2 assimilation rate [0..100 kg/ha/hr, R] as function of development stage [0..2 -, R]
                 AMAX (maximum 15 records)
          DVS
 AMAXTB =
           0.00 70.000
           1.25 70.000
           1.50 63.000
           1.75 49.000
           2.00 21.000
* End of table
```

```
* List reduction factor of AMAX [-, R] as function of average day temp. [-10..50 C, R]
         TAVD
              TMPF (maximum 15 records)
 TMPFTB =
         0.00 0.010
         9.00 0.050
        16.00
              0.800
        18.00
              0.940
        20.00 1.000
        30.00
              1.000
        36.00 0.950
        42.00
              0.560
* End of table
* List reduction factor of AMAX [-, R] as function of minimum day temp. [-10..50 C, R]
         TMNR
                TMNF (maximum 15 records)
 TMNFTB =
         5.00 0.000
         8.00
              1.000
* End of table
*************************************
* Part 6: Conversion of assimilates into biomass
 CVL
       = 0.6800 ! Efficiency of conversion into leaves,
                                                          [0..1 kg/kg, R]
 CV0
       = 0.6710 ! Efficiency of conversion into storage organs, [0..1 kg/kg, R]
       = 0.6900 ! Efficiency of conversion into roots,
 CVR
                                                          [0..1 \text{ kg/kg, R}]
 CVS
       = 0.6580 ! Efficiency of conversion into stems,
                                                          [0..1 kg/kg, R]
*****************
* Part 7: Maintenance respiration
 Q10
       = 2.0000 ! Rel. increase in respiration rate with temperature, [0..5 /10 C, R]
 RML
        = 0.0300 ! Rel. maintenance respiration rate of leaves, [0..1 kgCH2O/kg/d, R]
       = 0.0100 ! Rel. maintenance respiration rate of st. org.,[0..1 kgCH20/kg/d, R]
 RMO
 RMR
        = 0.0150 ! Rel. maintenance respiration rate of roots, [0..1 kgCH20/kg/d, R]
        = 0.0150 ! Rel. maintenance respiration rate of stems,
                                                          [0..1 kgCH2O/kg/d, R]
* List reduction factor of senescence [-, R] as function of dev. stage [0..2 -, R]
               RFSE (maximum 15 records)
         DVS
 RFSETB =
         0.00
               1.00
         1.50
               1.00
         1.75
               0.75
         2.00
               0.25
* End of table
* Part 8: Partitioning
* List fraction of total dry matter increase partitioned to the roots [kg/kg, R]
* as function of development stage [0..2 -, R]
         DVS
                     (maximum 15 records)
                FR
 FRTB =
         0.00
               0.40
         0.10
               0.37
         0.20
               0.34
         0.30
               0.31
         0.40
               0.27
         0.50
               0.23
         0.60
               0.19
         0.70
               0.15
         0.80
               0.10
         0.90
               0.06
         1.00
               0.00
         2.00
               0.00
* End of table
* List fraction of total above ground dry matter incr. part. to the leaves [kg/kg, R]
* as function of development stage [0..2 -, R]
```

```
DVS
                FL
                    (maximum 15 records)
 FLTB =
          0.00
                0.62
          0.33
                0.62
          0.88
                0.15
          0.95
                0.15
          1.10
                0.10
          1.20
                0.00
          2.00
                0.00
* End of table
* List fraction of total above ground dry matter incr. part. to the stems [kg/kg, R]
* as function of development stage [0..2 -, R]
          DVS
                FS (maximum 15 records)
 FSTB =
          0.00
                0.38
          0.33
                0.38
          0.88
                0.85
          0.95
                0.85
          1.10
                0.40
          1.20
                0.00
          2.00
                0.00
* End of table
* List fraction of total above ground dry matter incr. part. to the st. organs [kg/kg, R]
* as function of development stage [0..2 -, R]
          DVS
                FΩ
                     (maximum 15 records)
          0.00 0.00
 FOTB =
          0.95
                0.00
          1.10
                0.50
          1.20
                1.00
          2.00
                1.00
* End of table
**************************************
* Part 9: Death rates
 PERDL = 0.030 ! Maximum rel. death rate of leaves due to water stress [0..3 /d, R]
* List relative death rates of roots [kg/kg/d] as function of dev. stage [0..2 -, R]
         DVS
                RDRR
                       (maximum 15 records)
 RDRRTB =
        0.0000 0.0000
         1.5000 0.0000
         1.5001 0.0200
         2.0000 0.0200
* End of table
* List relative death rates of stems [kg/kg/d] as function of dev. stage [0..2 -, R]
                RDRS
                      (maximum 15 records)
 RDRSTB =
         0.0000 0.0000
         1.5000 0.0000
         1.5001 0.0200
         2.0000 0.0200
* Part 10: Crop water use
* -- Part 10a: Oxygen stress -----
* Switch for oxygen stress:
 SwOxygen = 1
                 ! 1 = Oxygen stress according to Feddes et al. (1978)
                  ! 2 = Oxygen stress according to Bartholomeus et al. (2008)
* If SwOxygen = 1, specify:
                    ! No water extraction at higher pressure heads, [-100..100 cm, R]
 HITM1 =
            -10.0
 HLIM2U =
             -25.0
                     ! h below which optimum water extr. starts for top layer, [-1000..100 cm, R]
```

```
HLIM2L =
            -25.0
                    ! h below which optimum water extr. starts for sub layer, [-1000..100 cm, R]
* If SwOxygen = 2, specify:
                 = 2.8d0
                                ! Relative increase in microbial respiration at temperature increase
  Q10_microbial
of 10 °C [1.0..4.0 -, R]
 Specific_resp_humus = 1.6d-3
                                ! 2.258d-4 ! Respiration rate of humus at 25 ºC [0.0..1.0 kg O2/kg
C/d, R]
 SRL
                    = 151375.d0 ! Specific root length [0.d0..1.d10 m root/kg root, R]
  SwRootRadius
                    = 2
                               ! Switch for calculation of root radius
                                      ! 1 calculate root radius
                                      ! 2 root radius given in input file
* If SwRootRadius = 1, specify:
                    = 0.075d0
  Dry_mat_cont_roots
                                    ! Dry matter content of roots [0..1.0 -, R]
                                    ! Air filled root porosity [0..1.0 -, R]
  Air_filled_root_por
                       = 0.05d0
  Spec_weight_root_tissue = 1.0d3
                                     ! Specific weight of non-airfilled root tissue [0.d0..1.d5 kg
root/m3 root, R]
                       = 4.175d-10 ! Variance of root radius [0.d0..1.d0 -, R]
 Var a
* If SwRootRadius = 2, specify:
 Root_radius02 = 0.00015d0
                                   ! meter! root radius for oxygen stress module
* -- Part 10b: Drought stress -----
* Switch for drought stress:
                   ! 1 = Drought stress according to Feddes et al. (1978)
 SwDrought = 1
                   ! 2 = Drought stress according to De Jong van Lier et al. (2008)
* If SwDrought = 1, or in case of irrigation scheduling, specify:
 HLIM3H = -20.0! h below which water uptake red. starts at high Tpot, [-10000..100 cm, R]
  HLIM3L =
             -20.0
                     ! h below which water uptake red. starts at low Tpot, [-10000..100 cm, R]
                   ! No water extraction at lower pressure heads, [-16000..100 cm, R]
 HLIM4 = -4000.0
  ADCRH =
              0.5 ! Level of high atmospheric demand, [0..5 cm/d, R]
  ADCRI =
               0.1 ! Level of low atmospheric demand, [0..5 cm/d, R]
* hidden option : (0.3 is default value after Jarvis for moderate drought compensation)
 ALPHACRIT = 0.7
                   ! Criticial stress index for compensation of root water uptake [0.2 .. 1.0 -,
R1
* If SwDrought = 2, specify:
 WILTPOINT = -20000.0 ! Minimum pressure head in leaves, [-1.0d8..-1.0d2 cm, R]
              1.03d-4 ! Conductance in the path from leaf to root xylem [1.0d-10..1.0d0 /d, R]
  KSTEM =
                0.02 ! Xylem radius, [0.0001..1 cm, R]
0.05 ! Root radius, [0.0001..1 cm, R]
  RXYLEM =
  ROOTRADIUS =
  KROOT =
              3.5d-5 ! Radial hydraulic conductivity of root tissue [1.0d-10..1.0d10 cm/d, R]
  ROOTCOEFA =
                 0.53 ! Defines relative distance at which mean soil water content occurs, [0..1.0 -,
  SWHYDRLIFT =
                   0 ! Switch for possibility hydraulic lift in root system, [N=0, Y=1]
 ROOTEFF =
                  1.0 ! Root system efficiency factor [0..1.0 -, R]
                  1.0 ! Step between values of hroot and hxylem in iteration cycle [0.d0..10.d0 cm,
 STEPHR
R]
 CRITERHR =
                   0.001 ! Maximum difference of Hroot between iterations; convergence criterium
[0.d0..10.d0 cm, R]
                    0.001 ! Maximum absolute difference between simulated and calculated potential
transpiration rate (1.0d-5..1.0d-2 cm/d, R)
* Part 11: salt stress
* Switch salinity stress
  SWSALINITY = 0 ! 0 = No salinity stress
                ! 1 = Maas and Hoffman reduction function
                ! 2 = Use osmotic head
* If SWSALINITY = 1, specify threshold and slope of Maas and Hoffman
  SALTMAX = 3.0 ! Threshold salt concentration in soil water [0..100 mg/cm3, R]
  SALTSLOPE = 0.1 ! Decline of root water uptake above threshold [0..1.0 cm3/mg, R]
* If SWSALINITY = 2, specify:
 SALTHEAD = 624.0 ! Conversion salt concentration (mg/cm3) into osmotic head (cm) [0..1000.0
cm/(mg/cm3), R]
* Part 12: interception
```

```
* For agricultural crops apply interception concept of Von Hoyningen-Hune and Braden
 SWINTER = 1 ! Switch for rainfall interception method:
               ! 0 = No interception calculated
               ! 1 = Agricultural crops (Von Hoyningen-Hune and Braden)
               ! 2 = Trees and forests (Gash)
 COFAB = 0.25 ! Interception coefficient, corresponding to maximum interception amount [0..1 cm, R]
              ******************************
* Part 13: Root density distribution and root growth
 RDI
             5.00 ! Initial rooting depth, [0..1000 cm, R]
 RRI
             2.20 ! Maximum daily increase in rooting depth, [0..100 cm/d, R]
            75.00 ! Maximum rooting depth crop/cultivar, [0..1000 \text{ cm, R}]
 RDC
* List root density [0..100 cm/cm3, R] as function of relative rooting depth [0..1 -, R]:
* In case of drought stress according to Feddes et al. (1978) (SWDROUGHT = 1), relative root density (-
) is sufficient
    Rdepth Rdensity
                           ! (maximum 11 records)
 RDCTB =
0.0,1.000
0.1.0.741
0.2,0.549
0.3,0.407
0.4,0.301
0.5,0.223
0.6,0.165
0.7,0.122
0.8,0.091
0.9,0.067
1.0,0.050
* End of table
* Expert-option for rooting depth limitation by relative dry matter increase (dmi/dmipot)
* (default = no limitation: SWDMI2RD = 0; with limitation: SWDMI2RD = 1)
  SWDMT2RD = 1
**********************************
*** MANAGEMENT SECTION ***
*** NITROGEN SECTION ***
** Nitrogen use
* Data from: Linutl4, http://models.pps.wur.nl/models
                     param values from MAG202.DATo
      reference:
                   Wolf, J. (2012). Users guide for LINTUL4 and LINTUL4V:
                   Simple generic model for simulation of crop growth under
                   potential, water limited and nitrogen limited conditions.
                   WUR-PPS report (Vol. 4).
                   ! max. relative death rate of leaves due to N stress
RDRNS
        = 0.05
DVSNLT
       = 1.3
                   ! development stage above which no crop nitrogen uptake does occur
DVSNT
        = 0.8
                  ! development stage above which nitrogen translocation to storage organs does occur
FNTRT
        = 0.15
                   ! nitrogen translocation from roots as a fraction of total N amount translocated
from leaves and stems
                  ! optimal N concentration as fraction of maximum N concentration
FRNX
        = 0.5
I RNR
        = 0.50
                   ! maximum N concentration in roots as fraction of maximum N concentration in leaves
                   ! maximum N concentration in stems as fraction of maximum N concentration in leaves
LSNR
        = 0.50
NLAI
         = 1.0
                      ! coefficient for the reduction due to N stress of the LAI increase (during
juvenile phase)
NLUE
        = 1.1
                   ! coefficient for the reduction of RUE due to Nitrogen stress
NMAXSO
        = 0.05
                    ! maximum N concentration (= 1.6*min. N conc.) in storage organs [kg N kg-1 dry
biomass]
                   ! coefficient for the effect of N stress on leaf biomass reduction
NPART
NSIA
                   ! coefficient for the effect of N stress on SLA reduction
        = 0.5
RNFLV
        = 0.0053
                   ! residual N fraction in leaves [kg N kg-1 dry biomass]
RNFST
        = 0.0027
                   ! residual N fraction in stems [kg N kg-1 dry biomass]
RNFRT
        = 0.0027
                  ! residual N fraction in roots [kg N kg-1 dry biomass]
TCNT
        = 10.0
                  ! time coefficient for N translocation to storage organs [days]
                 ! fraction of crop nitrogen uptake by biological fixation [-]
NFIXE
        = 0.0
NMXI V
        = 0.0, 0.06, ! maximum N concentration in leaves as function of development stage [kg N kg-
1 dry biomass]
```

0.4, 0.04, 0.7, 0.03, 1.0, 0.02,

```
2.0, 0.022,
          2.1, 0.022
***********************************
* Harvest losses of organic matter
FraHarLosOrm_lv = 0.2
                     ! fraction harvest losses of organic matter from leaves
                                                                                      [0.0..1.0
kg.kg-1 DM, R]
FraHarLosOrm_st = 0.1 ! fraction harvest losses of organic matter from stems
                                                                                      [0.0..1.0
kg.kg-1 DM, R]
FraHarLosOrm_so = 0.01 ! fraction harvest losses of organic matter from storage organs [0.0..1.0
kg.kg-1 DM, R]
***********************************
* Part 3: Management, other than mowing, grazing, irrigation, e.g. pests,diseases,nutrients,etc..
flpotrelmf = .false. ! Flag indicating calculation of attainable yield instead of theoretical
potential yield
relmf = 0.90
                   ! relative Management factor to reduce crop growth [0..1.0 [-], R]
** CO2-impact:
    correction of photosynthesis as a function of atmospheric CO2 concentration (-)
    correction of radiation use efficiency as a function of atmospheric CO2 concentration (-)
    correction of transpiration as a function of atmospheric CO2 concentration (-)
FLCO2 = .FALSE.
                   ! Switch/flag for application of CO2 correction [Y=.TRUE., N=.FALSE.]
*** IRRIGATION SCHEDULING SECTION ***
*********************************
* Part 1: General
 SCHEDULE = 0 ! Switch for application irrigation scheduling [Y=1, N=0]
* If SCHEDULE = 0, no more information is required in this input file!
* If SCHEDULE = 1, continue ....
 STARTIRR = 30 3 ! Specify day and month after which irrigation scheduling is allowed [dd mm]
 ENDIRR = 31 10 ! Specify day and month after which irrigation scheduling is NOT allowed [dd mm]
 CIRRS = 0.0
                ! solute concentration of scheduled irrig. water, [0..100 mg/cm3, R]
                ! Switch for type of irrigation method:
 ISUAS = 0
                ! 0 = sprinkling irrigation
                ! 1 = surface irrigation
* Specify pressure head at field capacity
* required for timing options TCS = 2, 3, or 4 and depth option DCS = 1, else dummy
 phFieldCapacity = -100.0 ! soil hydraulic pressure head [-1000.0 .. 0.0,cm, R]
***********************************
************************************
* Part 2: Irrigation time criteria
*** Choose one of the following 5 timing options:
 TCS = 5 ! Switch, timing criterion [1..6, I]]
           TCS = 1
                   : Daily Stress
           TCS = 2
                    : Depletion of Readily Available Water
                   Depletion of Totally Available WaterDepletion Water AmountPressure head or moisture content
           TCS = 3
!
           TCS = 4
           TCS = 5
           TCS = 6 : Fixed weekly irrigation, rootzone to field capacity
```

```
*** Daily stress criterion (TCS = 1)
* If TCS = 1, specify mimimum of ratio actual/potential transpiration Trel [0..1, R],
* as function of development stage DVS_tc1 [0..2, R], maximum 7 records:
 DVS_tc1 Trel
     0.0 0.95
     2.0 0.95
* End of table
*** Depletion of Readily Available Water (TCS = 2)
* If TCS = 2, specify minimal fraction of readily available water RAW [0..1, R],
* as function of development stage DVS_tc2 [0..2, R], maximum 7 records:
  DVS_tc2 RAW
     0.0 0.95
      2.0 0.95
* End of table
*** Depletion of Totally Available Water (TCS = 3)
* If TCS = 3, specify minimal fraction of totally available water TAW [0..1,\ R],
* as function of development stage DVS_tc3 [0..2, R], maximum 7 records:
  DVS_tc3 TAW
     0.0 0.50
      2.0 0.50
* End of table
*** Depletion Water Amount (TCS = 4)
* If TCS = 4, specify maximum amount of water depleted below field cap. DWA [0..500 mm, R],
* as function of development stage DVS_tc4 [0..2, R], maximum 7 records:
  DVS_tc4 DWA
     0.0 40.0
     2.0 40.0
* End of table
* Pressure head or Moisture content (TCS = 5), specify
              ! Switch, use either pressure head (PHORMC = 0) or water content (PHORMC = 1)
  DCRIT = -30.0! Depth of the sensor [-100..0 cm, R]
* Also specify critical pressure head [-1d6..-100 cm, R] or moisture content [0..1 cm3/cm3, R] as
function of crop development stage
  DVS tc5 Value tc5
            -1000.0
     0.0
     2.0
            -1000.0
* End of table
* In case TCS = 5, over-irrigation can be applied if the salinity concentration exceeds a threshold
salinity
* Switch for over-irrigation:
  SWCIRRTHRES = 0
                  ! 0 = No over-irrigation
                    ! 1 = Apply over-irrigation
* If SWCIRRTHRES = 1, specify:
  CIRRTHRES = 8.0
                      ! Threshold salinity concentration above which over-irrigation occurs [0..100
mg/cm3, R]
  PERIRRSURP = 10.0 ! Over-irrigation as percentage of the usually scheduled irrigation depth [0..100
* In case TCS = 6, specify:
* Fixed weekly irrigation, root zone back to field capacity (TCS = 6), specify
* Threshold value for weekly irrigation; only irrigate when soil water deficit in root zone is larger
than threshold
  IRGTHRESHOLD = 1.0
                          ! threshold value [0..20 mm, R]
* Switch for minimum time interval between irrigation applications
                  ! 0 = no minimum time interval
  TCSFTX = 0
                  ! 1 = define minimum time interval
* If TCSFIX = 1, specify:
  IRGDAYFIX = 7
                  ! Minimum number of days between irrigation applications [1..366 d, I]
```

\*

```
**********************************
* Part 3: Irrigation depth criteria
*** Choose one of the following 2 options for irrigation depth:
* Next line is required for Swap303 - swap3177
 DCS = 1
              ! Switch, depth criterion [1..2, I]]
                DCS = 1 : Back to Field Capacity
DCS = 2 : Fixed Irrigation Depth
*** Back to Field Capacity (DCS = 1)
* If DCS = 1, specify amount of under (-) or over (+) irrigation dI [-100..100 mm, R],
* as function of development stage DVS_dc1 [0..2, R], maximum 7 records:
  DVS_dc1 dI
    0.0 10.0
2.0 10.0
* End of table
*** Fixed Irrigation Depth (DCS = 2)
* If DCS = 2, specify fixed irrigation depth FID [0..400 mm, R],
* as function of development stage DVS_dc2 [0..2, R], maximum 7 records:
 DVS_dc2 FID
     0.0 60.0
     2.0 60.0
* End of table
*** Select (optional) limitations of irrigation depth:
  dcslim = 0 ! Switch, limited irrigation depth [0=No, 1=Yes] [0..1, I]
* If dcslim = 1, specify:
 irgdepmin = 0.0
                  ! minimum irrigation depth [0.0d0 .. 100.0d0, mm, I]
  irgdepmax = 0.0
                        maximum irrigation depth [irgdepmin .. 1.0d7, mm, I]
* End of .crp file !
```