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Towards effective land surface parameters for use with SVAT models: the use of similarity scaling and inversion techniques.

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1. Introduction

Determining the spatial and temporal variability in land surface characteristics and processes over large areas and long time periods is a difficult task, and considerable effort has been put into gaining experience and deriving appropriate models to deal with this challenge. However, despite improvements in prediction of the surface energy balance through the use of remote sensing data, there remains the lack of appropriate measurements and prediction methods for surface fluxes and soil moisture over a range of space and time scales.

These difficulties are apparent in analyses of data collected during multidisciplinary experiments such as HAPEX or FIFE: whereas a certain level of accuracy of the surface fluxes was achieved using vegetation indices and thermal infrared measurements, little new insight was gained about subjects such as water redistribution at the regional scale or multi-scale water storage status and dynamics.

Most of the models dealing with the soil water balance have a common energy balance representation, but differ significantly in their soil component and their representation of the spatial variability and the lateral flow. Because of the lack of spatial validation of these schemes, the computational cost seems to be the only criterion for preferring one scheme over another. A commonly used approach is to use simple models with « bulk » parameters accounting for strong correlations between basic parameters involved in the physical processes. This is illustrated by the use of a potential evaporation term across the catchment to capture the variability associated with the surface energy balance (albedo, LAI...), and the use of a bulk soil moisture content over a specific « hydrologically active » depth to capture the variability due to the soil moisture state (see Kim and Stricker, 1996).

Various Soil-Vegetation-Atmosphere Transfer (SVAT) schemes have been developed for use with for General Climate Models (GCMs) and Numerical Weather Prediction Models (NWPMs). However their weakest component remains their link with the lower boundary. SVAT models face various difficulties which include: (1) comparable complexity between system components; (2) scaling incongruities between atmospheric, hydrological and terrestrial components; and (3) validation of SVATs at appropriate space and time scales.

The need for improved characterisation of soil and landsurface properties at regional and global scales is generally recognised. This involves aggregation over heterogeneous surfaces. SVATs approach landsurface heterogeneity and subgrid variability either in a lumped fashion (with single effective, aggregated parameter values) or in the distributed fashion of a tile approach (with multiple optimised parameter sets or even multiple optimised sub-models, combined with the use of weighted averages).

The aggregation of above-ground vegetation parameters like LAI and soil cover may be based on simple linear averaging weighted by fractional areas. On the other hand canopy stomatal resistance may require a weighted harmonic mean: the optimal aggregation method will depend on actual distribution of resistances: low resistance values require harmonic mean; high resistance values need a linear average. Logarithmic averaging at the blending height is used for aerodynamic roughness

The aggregation of soil hydraulic parameters has been approached with various scaling techniques including dimensional analysis, similar media theory, and stochastic modelling. However it is not clear what an "areal average hydraulic property" really means. The questions is whether an heterogeneous soil may be treated as an equivalent "homogeneous" system with a set of effective properties.In this paper we will discuss similar media scaling and inverse modelling. Similar media scaling results in reference (i.e. average) value of soil hydraulic parameters and first order statistics of distribution of scaling factors. It is easy to use on large scales but has hardly been tested in GCM applications. Inverse modelling is very data intensive and hence difficult to use on a large scale. In catchment hydrology inverse modelling uses integral catchment data (e.g. river discharges or areal fluxes) with a hydrological model to arrive at an area-representative set of soil hydraulic parameters. Both methods are limited to a <u>single</u> textural soil class. Across textural classes, one may use area-average soil hydraulic characteristics from routinely available data on soil texture and the related soil-physical and soil-chemical data.

This paper has four parts. In Section 2 of this paper we draw some conclusions from recent simulation studies in the Lockyersleigh catchment in SE Australia with SiSPAT, a one-dimensional SVAT model. These studies had two broad aims. The first objective was to compare results obtained with deterministic and stochastic versions of SiSPAT with soil moisture content observations and with limited airborne flux measurements (Boulet *et al.*,1995ab; Boulet and Kalma, 1997). The second objective (see Boulet and Kalma, 1998; Boulet *et al.* 1999) was to use SiSPAT in a study of the impact of spatial variability in soil and land surface parameters on regional-scale water balance components and to investigate the use of effective landsurface parameters based on recently described hydrometeorological aggregation rules.

Section 3 addresses the use of inverse modelling with a SVAT scheme and areal estimates of surface fluxes and/or soil moisture data to obtain effective, mesoscale soil hydraulic parameters. The catchment-scale study by Feddes *et al.* (1993b) is summarised in which soil hydraulic properties are estimated with the dynamic one-dimensional soil-water-vegetation model SWATRE. This will point at the potential of combining large-scale inverse modelling of unsaturated flow with remotely sensed areal evaporation and/or areal surface soil moisture.

SVATs are usually over-parameterised and SVAT parameters are highly variable in space and difficult to measure. Significant uncertainty must therefore be associated with SVAT parameterisation. The last section of the paper provides an illustration of the uncertainty in SVAT parameterisation which results in predictive uncertainty of energy heat fluxes. To reduce this uncertainty SVAT models typically require calibration against measured fluxes. However, the complexity of these models prohibits the identification of a unique parameter set. Successful remote measurement of fluxes would provide additional information with which to calibrate SVAT models. In this section we investigate the potential utility of thermal signatures of the land surface through the application of the TOPUP-SVAT model. The results indicate that while significant uncertainty must always be associated with remote measures of the land surface response, a time series of thermal data collected over a dry-down period, can be usefully employed to provide improved parameterisation of SVAT constructs.

2. Simulation studies with SiSPAT at Lockyersleigh, Australia

SiSPAT (see Braud, 1996) is a one-dimensional SVAT model (see Figure 1), which is forced with a climatic series of air temperature, humidity, wind speed, incoming solar and long-wave radiation and rainfall. In the soil SiSPAT solves coupled heat and mass transfer equations for temperature T and matric pressure head h. The model uses the formulations of Milly (1982) to calculate liquid and vapor transfers in vertically heterogeneous soils.

The upper boundary conditions are obtained by the solution of the soil-plant-atmosphere interface, which results in the surface soil heat and mass fluxes and the surface matric pressure head h_1 and temperature T_1. If saturation of the surface occurs, the matric pressure head is set to zero and surface runoff is calculated from the mass balance equation. Bare soil and vegetation are considered separately in a two-source model (see Taconet *et al.*, 1986). Five equations can be written: energy budget over bare soil and vegetation; continuity of the sensible and latent heat fluxes through the canopy and continuity of the surface mass flux at the soil surface. Leaf temperature T_v, canopy temperature T_{av}, canopy specific humidity θ_{av}, soil surface temperature T_1 and surface matric pressure head h_1 can then be calculated and the surface energy and mass fluxes can be obtained.

In the soil, a root extraction term is included and modelled with a resistance network. The assumption that the total root water extraction is equal to the plant transpiration allows for the computation of the leaf water pressure head h_f which is used to compute the stomatal resistance water stress function. The incoming energy is partitioned between bare soil and vegetation through a shielding factor σ_f (Taconet *et al.*, 1986).

In order to solve moisture and heat transfer equations in the soil, functions are needed to relate matric pressure head and hydraulic conductivity to volumetric water content θ, yielding $h(\theta)$ and $K(\theta)$. Introducing a relative saturation term S_e, where

$$S_e = (\theta - \theta_{res}) / (\theta_{sat} - \theta_{res}) \quad (1)$$

the required functions are described by Van Genuchten (1980) as:

$$S_e = \{ 1 + (h/h_g)^n \}^{-m} \quad \text{with } m = 1 - (2/n) \quad (2)$$

$$K = K_{sat} (S_e)^2 [1 - \{1-(S_e)^{1/m}\}^m] \quad (3)$$

The closed-form analytical expressions (1), (2) and (3) contain one shape parameter m and four scale parameters: h_g as scale factor in the retention curve expression, residual water content θ_{res}, saturated water content θ_{sat}, and hydraulic saturated conductivity K_{sat}. The shape parameter m is related to the texture of the soil (sandy loam and clay loam for this study) and the scale parameters depend mainly on the structure of the soil (compaction of the aggregates and of the soil, macropores, roots, etc). The spatial variability of the scale parameters is usually larger than that of the shape parameters. Non-linear least-squares curve-fitting techniques have been used to estimate the various parameters from measured h-Θ data. [The equations show that the hydraulic conductivity function may solely be obtained from a measured K_{sat} and the shape parameter m obtained from fitting water retention data to (2)]

SVAT modelling has rarely been at the landscape scale in order to take into account the spatial variability of land cover, pedology and topography. Boulet and Kalma (1997) have used the one-dimensional SiSPAT model for a 60 day period in the 27 km^2 Lockyersleigh catchment in SE Australia with (1) a stochastic approach in which they assume that a statistical distribution of a critical catchment parameters such as soil moisture storage capacity, can explain the major part of catchment variability and will provide an average value for the entire catchment; and (2) a deterministic approach, in which the catchment is subdivided into 40 "homogeneous" subregions which are only linked by surface runoff. Output obtained with the stochastic approach for the catchment as a whole is compared with results obtained with a network of soil moisture measurements and a semi-distributed hydrology model (VIC/PATCHY, see below) in Figure 2 which shows a comparison of a catchment scale soil moisture index w/w_c. The VIC model (see Wood *et al.*, 1992; Kalma *et al.*, 1995) assumes a variable bucket representation and relates spatial variability in soil moisture storage capacity for homogeneous soil profiles to differences in soil depth and the porosity. It is shown that SiSPAT reproduces the evolution of the hydrological state of the landscape reasonably well.

With the deterministic approach SiSPAT results based on 40 subregions have been compared with the results obtained with a distributed -parameter hydrological model TOPOG-IRM which simulates the water balance across the three-dimensional catchment using 2000 cells. Table 1 shows a summary of cumulative catchment water balance components obatained with SiSPAT and TOPOG-IRM, whereas Figure 3 compares cumulative catchment evaporation in time as predicted with the two models.

Boulet *et al.* (1995ab) and Boulet and Kalma (1997) show detailed results with "first guess" parameters. They obtained reasonable agreement with seven sets of (total) soil moisture content observations during a 60-day period and with airborne flux measurements on three days.

A study of the spatial and temporal variability of soil moisture in the Lockyersleigh catchment in SE Australia was reported by Kalma and Boulet (1998). They simulated soil moisture content with SiSPAT and the stochastic hydrological model (VIC) and compared these simulations with soil moisture measurements made with NMM equipment in 41 locations on 35 days throughout a 437 day period. The specific aims of their study were: (1) to compare the simple VIC model which has been calibrated using streamflow observations and the detailed SiSPAT model which requires many parameters (and thus, strictly speaking, can not be calibrated) and to compare model simulations with soil moisture measurements made at a large number of locations; (2) to investigate if most of the spatial variability of the soil moisture dynamics can be explained by accounting for the depth of the top permeable soil layer and an accurate initial soil moisture profile; and (3) to verify what level of heterogeneity of the soil moisture can be explained by a variable sandy layer depth.

Kalma and Boulet (1998) show how both the SiSPAT and VIC models yield simulations of the water dynamics for an array of vertical columns, i.e. by applying climate forcing to a number of unconnected soil profiles which represent an array of NMM tubes. The stochastically distributed, one-dimensional SiSPAT model (which is not calibrated) transfers any runoff instantaneously to the catchment outlet. SiSPAT does not consider any subsurface runoff nor does it consider the development of a saturated zone. The results indicate that time trends for small, medium and large storage capacities show reasonable agreement between observations and simulations for small storage capacities but the agreement is less satisfactory for larger storage capacities.

The w/w_c ratio is a catchment scale wetness index which incorporates all measurement tubes. The results of Figure 5 are encouraging for the calibrated VIC but indicate that an uncalibrated SiSPAT misrepresents very dry and very wet periods. This is very likely more due to inadequate estimation of the soil hydraulic parameters than to errors in vegetation parameters. SiSPAT gave lower quality results than the VIC model. However, the good results with the VIC mean that it captures the strongly one-dimensional (vertical) nature of the water fluxes at and near the land surface. The relevance of its use over the use of a simple Manabe bucket with « effective » parameters remains dependent on the generality of two parameters for distribution of soil moisture storage (b and s_{min}; see Kalma *et al.*, 1995). However, the physical significance of these « bulk » parameters is difficult to determine. This concern is a major drawback for the use of the VIC model, compared with the use of SiSPAT. Although SiSPAT works less successfully with first-guess parameters, it does not require information on the (spatial distribution of the) storage capacity. Finally, it should be noted that both models were unable to accurately simulate the major event when surface and subsurface runoff occurred, which stresses the need to take into account the lateral patterns of moisture flow when rainfall intensity is strong enough to saturate the soil above the impermeable layer.

In another study (see Boulet and Kalma, 1998; Boulet *et al.* 1999) SiSPAT has been used to study the impact of spatial variability in soil and land surface parameters on regional-scale water balance components in the Lockyersleigh catchment. A statistical-dynamical approach was used to account for the spatial variability of selected parameters and to determine the seasonal evolution of the impact on the water budget. More specifically, that study addressed scaling techniques by applying the geometric similarity concept of Miller and Miller (1956) which is based on the similarity of two soils which are geometrically alike except for the scale of their internal porosities. The spatial variability in h-Θ-K characteristics can then be described by a scale factor α_x for site x which may be expressed as

$$\alpha_x = \lambda_x / \lambda_r \qquad (4)$$

where λ_x and λ_r are the (microscopic) characteristic length scales respectively of a soil at location x and of a reference soil, and where x=1, 2,....., X denotes individual locations. Scale factors relate soil hydraulic properties at each location to a representative mean or to reference curves. Variations in the soil water retention curve and the hydraulic conductivity function are therefore connected by the scale factor α.

According to Raats (1990) the following scaling rules may then be derived for soil moisture content Θ, pressure head h and hydraulic conductivity K

$$\Theta_x = \Theta_r \qquad (5)$$

$$h_x = \alpha_x^{-1}\, h_r \qquad (6)$$

$$K_x = \alpha_x^{2}\, K_r \qquad (7)$$

These equations imply that the soil water retention and hydraulic conductivity characteristics at given water content Θ at any location may be related to the mean Θ-h-K functions (i.e. the mean Θ_r, h_r and K_r values), and are of a general form:

$$\zeta_x = \alpha_x^{n}\, \zeta_r \qquad (8)$$

Kabat *et al.* (1997) note that for many variables in SVAT scheme parameterisations secondary scaling rules may be inferred from the form of the Darcy equation and the mass conservation equation. They provide values of n for several variables and parameters used to model water flow. Raats (1990) shows that the log-normal distribution of the scaling lengths λ implies that scaled water flow variables and parameters will also be log-normally distributed.

Examples of unscaled soil hydraulic characteristics obtained by laboratory measurements on undisturbed soil samples and the results when simultaneous similar media scaling is applied to all functions resulting in reference curves for soil water retention and hydraulic conductivity are shown in Figure 6.

Previous studies using other land-surfaces schemes (e.g. Avissar, 1995) and the studies of Boulet *et al.*(1995ab) and Boulet and Kalma (1997) have shown that critical parameters for the description of the water budget are the depth of the top sandy layer (A horizon) z_{sand}, the scale (θ_{sat}, K_{sat} and h_g) and shape (m) parameters of the water retention and hydraulic conductivity curves, the Leaf Area Index (LAI) and the minimum stomatal resistance (R_{stmin}).

Local field data and data obtained from extensive field work carried out in the Tablelands region of southern New South Wales and northern Victoria provided information on the distributions of these soil parameters (see Table 2 and Figure 7). The probability-density functions for a range of land surface characteristics were used to generate sensitivity patterns for evaporation, transpiration and runoff. The means of these univariate distributions of outputs yielded catchment-scale averages. The study also obtained catchment-scale evaporation estimates by running simulations with *aggregated* parameters obtained as statistical descriptors of parameter distributions. The difference between the catchment-scale averages and values obtained with aggregated parameters described the non-linear response of the model to spatial variability of the particular parameter. This study has provided examples of the impact of simulated spatial variability in land surface parameters on the four water budget components: evaporation from the soil surface, transpiration from the vegetation, total evaporation and runoff. *Local Deviation* values are used to develop sensitivity patterns for these four components for individual seasons and for the year as a whole. Figure 8 shows that large changes in sensitivity patterns are found between seasons.

A statistical method is used to investigate the effectiveness of using the arithmetic mean of an input parameter as an "effective parameter" in reproducing the average behaviour of the system. Results are encouraging in spring, autumn and winter, when the complexity of the interactions between different processes and the high frequency of rainfall is not very great. Differences (*Regional Deviations*) between average values and outputs based on arithmetic means of input parameters for these three seasons are of the same order of magnitude as the mass-balance uncertainty allowed by the computational constraints on time cost-efficiency. However, in summer Regional Deviations are considerable if the arithmetic mean of the distribution is used (see Figure 9).

Several *effective* parameters were investigated based on recently described hydrometeorological aggregation rule (see Figure 10). Aggregating rules based on median values of the input parameter improve the accuracy of the one-dimensional catchment-scale water budget simulation. However, several existing aggregation rules developed from simplified parameterizations (like the Penman-Monteith equations) do not adequately consider the analytical complexity of the model or, therefore, the possible interactions between the transfer phenomena. In this study, the rules derived for the minimum stomatal resistance R_{stmin} fail to reproduce the averaged water budget. The study showed significant differences in sensitivity patterns between individual parameters and between seasons. Runoff generation was highly non-linear and in turn affected all other surface fluxes. It was strongly affected by the spatial variability in the soil moisture storage capacity.

The work described by Boulet and Kalma (1998) and Boulet *et al.* (1999) may be extended in two areas. The first one is to derive effective parameters from the use of Taylor series expansion around the parameter mean. The second area is to recognize that the key parameters investigated in this study are not independent because strong associations may exist between soil, vegetation and topographic positions (see Band and Moore, 1995). Kim *et al.* (1997) presented a method to develop effective parameters that takes into account the parameter dependencies. Finally, we note that spatial rainfall variability has been neglected in this study. In drier environments, the impact of spatial and temporal rainfall variability on heat and mass exchange must also be investigated.

3. Inverse modelling to obtain effective, mesoscale soil hydraulic parameters

There is a need to parametrise and scale up heterogeneous soil hydrological processes. However scaling procedures are complicated by the non-linear behaviour of two basic characteristics of soil water flow: soil water retention and hydraulic conductivity. Sub-grid scale variability in soil parameters and soil moisture behaviour must be parameterised for use in mesoscale and large-scale climate models. It has been shown that inverse one-dimensional modelling may be used to estimate regional-scale *effective* soil hydraulic parameters. This requires the use of a physically-based model for vertical soil water movement that reacts to changes in boundary conditions, irrespective of spatial scale considered.

Soils have non-linear flow properties: strong non-linear relationships exist between moisture fluxes and hydraulic head gradients. Sudden changes in boundary conditions translate into gradual changes in water movement. Macroscopic flow properties consist of relationships between pressure head, soil water content and hydraulic conductivity.

Assuming that small-scale soil hydraulic property formulations can adequately describe large-scale hydraulic properties, then traditional small-scale soil physics may be employed to estimate areal vertical water movement at larger scales, i.e. by application of the one-dimensional Darcy/Richards (DR) flow equation. Through inverse modelling, effective soil hydraulic properties may be derived for an area as a whole using areal flow data (evapotranspiration, drainage, soil moisture changes). This would allow the area to be modelled for specified boundary conditions with a single simulation of a one-dimensional model. Thus spatial variability is averaged before simulations rather than afterwards. This approach therefore assumes scale invariance of the DR equation. It should be pointed out however (see Feddes *et al.*, 1993b) that there is no *theoretical* justification for the existence of effective parameters on the field scale.

Inverse modelling is widely used in groundwater hydrology (e.g. Wagner and Gorelick, 1986) and also in unsaturated soil water flow problems (Mantoglou and Gelhar,1987; Kool *et al.*, 1987; Mishra *et al.*, 1990). The resulting *effective* soil hydraulic parameters thus integrate micro-scale variability.

Feddes *et al.* (1993a) and Feddes (1995) discuss the potential of combining large-scale inverse modelling of unsaturated flow with remotely sensed areal evaporation and areal surface soil moisture. They describe lysimeter-scale and catchment-scale examples of estimation of soil hydraulic properties by the dynamic one-dimensional soil-water-vegetation model SWATRE/SWACROP.

SWATRE (Belmans *et al.*, 1983) is a numerical one-dimensional model developed to solve the DR equation for different soil depths based The model uses an implicit finite difference scheme and applies an explicit linearization of hydraulic conductivity (K_h) and soil water capacity C. A detailed description of the initial (i.e. Θ or h profile), upper (surface) boundary and lower boundary conditions has been given by Feddes *et* *al.* (1988). The model uses potential transpiration and potential soil evaporation as forcing functions. The iteration procedure within each time step allows for the calculation of all the terms of the soil water balance.

The catchment-scale study described by Feddes *et al.* (1993ab) and illustrated in Figure 11 investigated the feasibility of estimating effective soil hydraulic parameters for a 6.5 km2 catchment by inverse modelling. A total of 32 distributed soil samples were taken of the top 30cm soil layer and used to obtain h(Θ) and K(h) curves for each sample as well as a set of *reference curves* for water retention and soil hydraulic conductivity with a geometrically similar-media technique. These reference curves were described with the Mualem-Van Genuchten (MVG) conceptual model (Van Genuchten, 1980). In this study a log-normal distribution for scaling factors and a normal distribution for Θ_s were assumed. The reference curves and the distribution of scaling factors were used to generate soil hydraulic properties for 32 hypothetical bare soil "columns".

Numerical evaporation/infiltration experiments were then carried out with SWACROP/SWATRE for each of 32 soil "columns" for different sets of meteorological conditions and initial data which represent a reasonable range of field conditions. Outputs from the 32 experiments were used to calculate daily "areal" soil water content profiles and soil water fluxes.

With an inverse modelling approach SFIT (Kool and Parker, 1987) effective soil hydraulic curves for h(Θ) and K(Θ) were generated with several subsets of "areal" data (volumetric water content; cumulative evaporation and infiltration) for a single "effective" soil column representing the entire catchment. Different optimisation procedures may be used to ensure that model outputs closely match area averages values. The inverse problem is then formulated as a non-linear optimisation problem in which the function parameters are optimised by minimising a suitable objective function which expresses the discrepancy between observed and predicted response of system (see for example Kool and Parker (1988)).

The output of the SWATRE-runs with *effective parameters* were compared with the "areal average" resulting from averaging the output of simulations on the 32 soil columns. This was done for a range of meteorological forcing and initial data, and for various subsets including soil water content, cumulative evaporation and cumulative infiltration. The results obtained by Feddes *et al.* (1993ab) as shown in Figures 12 and 13 indicate that small scale soil physics can adequately describe large-scale hydrological phenomena.

The numerical experiments of Feddes *et al.* (1993ab) are reviewed by Kabat *et al.* (1997). They provide further detail on a verification experiment in which the best performing sets of inversely fitted parameters were validated on soil covered with grass for several years with conditions which fell outside the range over which the effective parameters were optimised. Area-average, effective parameterisation of soil hydraulic functions in combination with numerical solution of scale-invariant DR equation can work well in some cases, whereas reference soil hydraulic functions obtained through geometric similarity scaling performed well in all cases. It was concluded that the inverse technique provided *effective* soil parameters which performed well in predicting area-average evaporation and area averaged soil moisture fluxes such as subsurface runoff over a domain with a single textural soil type. Thus regional-scale *effective* soil hydraulic parameters may be obtained by inverse modelling in combination with a numerical solution of the scale invariant Darcy-Richards equation, on the basis of areal evaporation and surface soil moisture data. Such an approach envisages the use of remote sensing based, scale-integrating measurements of soil moisture and estimates of evaporation over large areas.

Kabat *et al.* (1997) emphasise that *effective* parameters refer to domains with the same textural soil type, whereas *aggregated* parameters refer to domains with several different textural soil types. Typical subgrids of mesoscale atmospheric models would usually comprise several textural (or pedological) soil types. Aggregated soils should, like effective soils, result in the same dynamic hydrological system, compared with an area average based on procedures which retain the soil variability.

Cosby *et al.* (1984) and Noilhan and Lacarrere (1995) introduced a soil aggregation procedure based on the observation that variability in soil hydraulic parameters could be related to variation in sand and clay fractional content. Kabat *et al.* (1997) describe a numerical experiment to test this soil aggregation procedure. They assumed that the mean values and variances of parameters of the Clapp and Hornberger (1978) exponential model (CH) for describing the soil's hydraulic characteristics are linearly dependent on soil texture, and used multilinear regression analysis to relate characteristics to sand and clay content to yield *aggregated* values of the CH parameters. Using a one-dimensional SVAT model (SWAP/MITRE) (Kabat *et al.*, 1997) concluded that aggregated soil parameters yielded reasonable good results for areal evaporation flux simulation but failed in the prediction of downward percolation and runoff.

4. Over-parameterisation of SVATs, parameter uncertainty, and the potential information content of thermal data.

Surface energy fluxes can vary significantly in space and time due to the variability in land surface properties. Recent studies have shown that characterising such properties is fraught with difficulties, as determining representative parameterisations is non-trivial due to our inability to accurately measure land surface properties. Where *measurement* of relevant model parameters cannot be achieved, parameters may often be identified through *calibration* to measured fluxes. However, SVAT models are typically over-parameterised with respect to the available calibration data, as the complexity of the models provides non-unique optimal parameter sets (Franks and Beven, 1997).

Franks (1999) has recently demonstrated that a major constraint of the calibration process is the quality of calibration data. Often calibration data do not display the full range of possible system dynamics and hence the informative content of the data may be limited. For example, one may collect three months of flux data, but if this period corresponds to a frequently wetted land surface where the surface vegetation is never moisture limited, then the collected data can contain no information related to a longer term drying of the land surface. It is therefore apparent that the robust calibration of SVAT models must only be achieved with data that display as much of the natural system dynamic as possible. This will necessitate routine measurements of the land surface behaviour over longer time periods than are typically collected through intensive field campaigns such as FIFE, ABRACOS and HAPEX. Remote thermal sensing provides one such possibility of obtaining additional calibration information.

Numerous schemes and methodologies have been proposed to provide estimates of land surface fluxes utilising thermal signatures derived from a variety of remote sensing platforms. However, deriving estimates of heat fluxes from thermal signatures alone, in common with SVAT models, is subject to uncertainty. To derive an instantaneous heat flux estimate, land surface parameters must be specified. Additional uncertainty must also be associated with such remote estimates due to the fact that thermal measurements are typically incommensurate with SVAT model variables and parameters (see Stewart *et al.*, 1998). Corrections must be applied to the raw radiance data to account for factors such as variable atmospheric effects, non-black body emissivity of the land surface, etc. As such, latent heat fluxes estimated in this way are subject to significant uncertainty through the requirement to parameterise the model which interprets the remote sensing. Significant uncertainty must be associated with the specification of all surface (aerodynamic) and sub-surface (hydrological) parameters. This uncertainty is already marked at the local patch (or plot) scale, and must be even greater when spatial variability of these parameters is considered. Whilst aerodynamic properties cannot be assigned without uncertainty, a degree of characterisation may be achieved through the specification of coarsely defined, uncertain ranges for each broad class of surface type. Additionally, a degree of uncertain correlation between parameters must also be expected – available moisture must be a function of rooting depth, which will in some manner be uncertainly linked to the vegetation height.

McCabe *et al.* (1999) have used combinations of feasible land surface characteristics associated with broadly defined vegetation types to parameterise the TOPUP-SVAT model of Beven and Quinn (1994). Uncertain parameter correlation will also permitted. This correlation couples individual model parameters to simplified functions of the canopy height of the surface type under consideration. The derived surface heat fluxes and thermal signatures are then analysed for unstressed vegetation conditions. This analysis is performed to reveal the uncertainty associated with surface fluxes estimated from a surface temperature measure and a specified land surface parameterisation.

Whilst marked uncertainty exists in the specification of land surface parameters, the actual *functional behaviour* of latent heat flux time series is relatively conservative – latent heat fluxes rarely exceed the input net radiation and hence daytime fluxes are typically constrained between zero and the net radiation (Franks and Beven, 1997; Beven and Franks, 1999). It has also been shown by Shuttleworth *et al.* (1989), Brutsaert and Sugita (1992) and Bastiaanssen *et al.* (1997) that the evaporative fraction $\Lambda = \lambda E/(\lambda E + H)$ as an indicator of energy partititoning is fairly constant during daylight hours. Furthermore, the observation of non-uniqueness of parameter sets in reproducing time series of heat fluxes may also be seen in a converse light – many distinct parameter sets, from very *different* parts of the parameter space, may produce the *same* function in terms of the temporal series of latent heat fluxes. The importance of this observation lies in the fact that if we wish to simulate time series of latent heat fluxes, then one need only identify the functional behaviour of the land surface. In terms of land surface flux behaviour in a drying period, differences in unstressed fluxes might be of secondary importance. Of more significance is the accurate simulation of how and when a surface reduces and stops evaporative losses, as this is more directly linked to the total available moisture store of the land surface (Franks, 1999). It is therefore expected that the *temporal pattern* of energy flux response will provide greater insight into the functional behaviour and appropriate parameter values than any single estimate of the instantaneous flux is capable of doing. By comparing the temporal pattern of thermal responses, one may therefore achieve robust characterisation of the land surface function as well as a degree of parameter tractability. This study therefore seeks to assess the potential utility of land surface thermal signatures in the identification of appropriate models of land surface flux behaviour.

TOPUP-SVAT (Beven and Quinn, 1994) is a simple SVAT model that represents the key physical processes controlling surface energy fluxes in a realistic but parametrically refined manner. Unlike other more complex SVAT constructs such as SiB, BATS and SiB2, TOPUP-SVAT requires a minimum of only eight parameters to be specified. The rationale for developing a simpler model structure is that simplicity is necessary to empirically validate the use of such SVAT models in the field. Limited calibration data are available for such purposes, again highlighting the significant parametric and predictive uncertainty existing in the calibration and evaluation of SVAT models. This problem is compounded for more complex models that are grossly over-parameterised with respect to the available calibration/evaluation data sets. The model incorporates the effects of near-surface stability conditions for the calculation of aerodynamic resistance and utilises the Penman-Monteith equation to predict latent heat fluxes.

McCabe *et al.* (1999) distinguish three classes of land surface cover: bare soil (sand), grass and trees. Parameter ranges for each of the variables of interest can be defined *a priori* based on physical relations, from experience or published literature.

Table 3 shows the distinct ranges of feasible parameter classes that have been assigned in this study to the different land surface/vegetation cover types. In order to investigate the thermal and evaporative response to these broad parameterisations of a simple SVAT model, multiple parameter realisations are required. To sample the 'likely' parameter space for each identified land surface cover type, 5000 individual parameter sets were constructed. It is important to note that this procedure treats parameters as *sets,* as all parameters are varied simultaneously. The randomly selected values for the individual parameters are then forwarded into the model as *a complete parameter set.* For each sampled parameter set, TOPUP-SVAT was initialised with a fully wetted root zone.

TOPUP-SVAT was then run with a long period of rainfall-free forcing data derived from the ABRACOS campaign, to investigate the dry-down behaviour of the within and between class responses of the various surface covers in terms of surface energy fluxes and thermal signatures. After definition of 5000 unique parameter sets for each cover type, the model was run for each of these multiple realisations over 1700 hourly time steps. In addition to the 5000 parameter sets associated with each land surface cover type, a single parameter set was selected for each cover type from the mid-point of the cover-specific parameter space. These unique parameter sets were then used to parameterise TOPUP-SVAT and were subsequently employed as *pseudo-observation records* for the associated surface cover. The temporal response of the derived temperature series was designated as the *'true' surface response* (as would have been obtained with remote sensing) against which the model predictions could be compared.

Figure 14 shows a plot of the modeled range of latent heat flux against the aerodynamic surface temperature calculated by TOPUP during *unstressed conditions*, extracted at the beginning of the runs comprising 1700 time steps. A distinct structure between the defined land covers can be observed. As expected, the soil displays the highest measures of instantaneous latent heat fluxes and surface temperatures, whereas the tree class shows the lowest instantaneous latent heat fluxes and lower aerodynamic temperatures. The plot also illustrates the relative uncertainty in estimating latent heat fluxes as a direct function of remotely sensed radiative surface temperatures. If one could accurately measure an appropriate aerodynamic surface temperature, the effect of parameter uncertainty is such that a large range of inferred latent heat fluxes is possible. It is therefore clear that parameter uncertainty prohibits the retrieval of instantaneous fluxes from surface temperature measures alone.

Surface temperatures are significantly sensitive to the land surface aerodynamic properties, however a recent sensitivity analysis of TOPUP-SVAT indicated that latent heat fluxes are relatively insensitive to aerodynamic properties given uncertainty in the other model parameter values (Franks *et al.*, 1997). Additionally, model predicted aerodynamic surface temperature is not the same as the remotely measured radiometric surface temperature, although the difference between the two is approximately constant over the typical range of temperatures (Huband and Monteith, 1986). Therefore, if one were to utilise the sensed surface temperatures, a significant error may be incorporated and any defined objective function may be inappropriately biased by marked sensitivity of the aerodynamic parameters.

In their study McCabe *et al.* (1999) seek to identify the *functional behaviour* of the land surface in terms of latent heat fluxes, through reference to the temporal changes of the surface thermal signature. To achieve this, the 'contending modelled thermal responses' were normalised relative to the observed (sensed) thermal sequence. The modeled thermal responses were scaled to the extreme temperatures of the 'observed' record, such that the modeled response matches the observed record at the positions of maximum and minimum temperature. The remaining temperatures are then fitted accordingly, using a simple linear equation to adjust values throughout the temporal series. The 'contending' model parameter sets were then evaluated with respect to the 'matching' to the observed sequence through an objective function based on sum of squared errors. The best 1% of model simulations (50 out of 5000) that reproduced the normalised temporal patterns of surface temperature were retained as 'acceptable' simulators of the (pseudo-) observed data. The retained acceptable parameter sets were then analysed in terms of the range of cumulative latent heat fluxes, time series of latent fluxes, and their constituent individual parameter values. This was achieved for both grass and tree land surface cover types.

Figure 15 shows cumulative likelihood plots for the pre- and post-conditioned randomly sampled parameter sets for grass and for trees. The solid line refers to the pre-conditioned (5000) parameter sets, whilst the dashed lines represent the cumulative likelihood of the (50) parameter sets deemed acceptable after comparison to the 'observed' thermal time series. These plots show the effect of the conditioning with respect to the relative constraint of two of the model parameters (SRMAX – available soil moisture storage; RSMIN – minimum surface resistance), and the cumulative latent heat flux over the period of simulation.

As can be seen from Figure 15, there is a marked distinction between the various parameter responses over the range of parameter simulations. SRMAX for the grass surface is well constrained within the parameter range. This is compared to SRMAX for the forest, which exhibits no significant behavioural response from the soil moisture storage. A similar trend is observed for RSMIN with the converse result of the forest parameter space becoming more highly constrained than is noticed for the grass cover. However, the latent heat response for both cover types reveals a constrained range of modelled flux predictions, despite the lack of constraint between the individual parameters. Hence, correct functional performance is achieved in both cases regardless of the different discrete parameter responses exhibited between the grass and tree covered surfaces.

Figure 16 shows the 95% uncertainty bounds of latent heat fluxes for the grass land-surface cover type. The solid lines refer to the upper and lower bounds of the latent heat fluxes of the 5000 random samples from the grass cover parameter ranges. As can be seen, large uncertainty must be associated with the predicted fluxes following the specification of any set of unique parameter values for this cover type. The dashed lines, however, represent the resultant predictive uncertainty following the conditioning of the parameter sets on the normalised temporal sequence of surface temperatures. As can be seen, the uncertainty envelope is drastically reduced relative to the un-conditioned parameterisations. It can be seen that at time step 430 (solid line), some realisations of the parameter space produce an ET flux of zero, indicating that the soil moisture store in the grass is at a minimum and that the surface exhibits conditions representative of a dry-down state. This situation is protracted for the normalised prediction (dashed line) which produces drydown conditions at time step 1030. This indicates that whilst gross uncertainty in instantaneous fluxes must be expected when inferred from a thermal measurement alone, a temporal series may be usefully employed in constraining this uncertainty.

This assessment of the utility of temporal series of thermal data in the estimation of land surface evapotranspiration has led to the following conclusions. The prediction of latent heat fluxes from absolute measures of surface temperatures (see Figure 14) was seen to be inherently uncertain. Through the analysis of a temporal series of latent heat fluxes, an enhanced prediction of the dry-down dynamics can be achieved. Additionally, the narrowing of the uncertainty bounds for the normalised temporal pattern allows an improved parameterisation of SVAT constructs to be achieved. This is important because SVAT models are generally over-parameterised with respect to the available data.

The dry-down dynamics of both grass and tree surface covers were examined in light of an artificial forcing and observation record. The enhanced reproduction of latent heat fluxes has been assessed using functional similarity between temporal responses as opposed to an instantaneous estimate derived from broadly defined parameter ranges. The problems related to atmospheric influences of emissivity and transmissivity affecting remotely sensed images are to some extent accounted for through adjusting the temporal series of temperature predictions. The simple linear normalisation process that is employed, allows the complication of correlating 'sensed' radiative temperatures and modelled aerodynamic temperatures to be addressed. Acknowledging that the difference between aerodynamic surface temperature and sensed radiative temperature is functionally similar, implementing a methodology that discriminates between parameter sets based on their temporal similarity to the observed temperature record will more closely reproduce that observed response.

The study of McCabe *et al.* (1999) relies on adequate provision of appropriate meteorological data. It should be noted that in certain applications this may not be readily available. However recent studies have indicated that the coupling of SVAT and Atmospheric Boundary Layer (ABL) models may allow improved estimates of aerodynamic temperature to be made. It is expected that the use of temporal patterns will provide the greatest insight when spanned across a period of wetting-up/drying-down dynamics. The importance of capturing this period from an unstressed to a stressed state is that it allows direct examination of vegetation response and the associated behavioural changes, thus facilitating a refinement of parameter specification.

The use of a time series of aerodynamic surface temperatures revealed appreciable insight into the dynamics of the dry-down phase over a variety of simulated surface covers. Inter-class parameter behaviour provided some useful insights into the controlling or more sensitive parameters in the SVAT model. The implementation of a conceptually simple normalising procedure and the associated recognition of multiple parameter set or non-unique solutions, facilitated a more improved and tightly constrained range of predictions for many of the model parameters.

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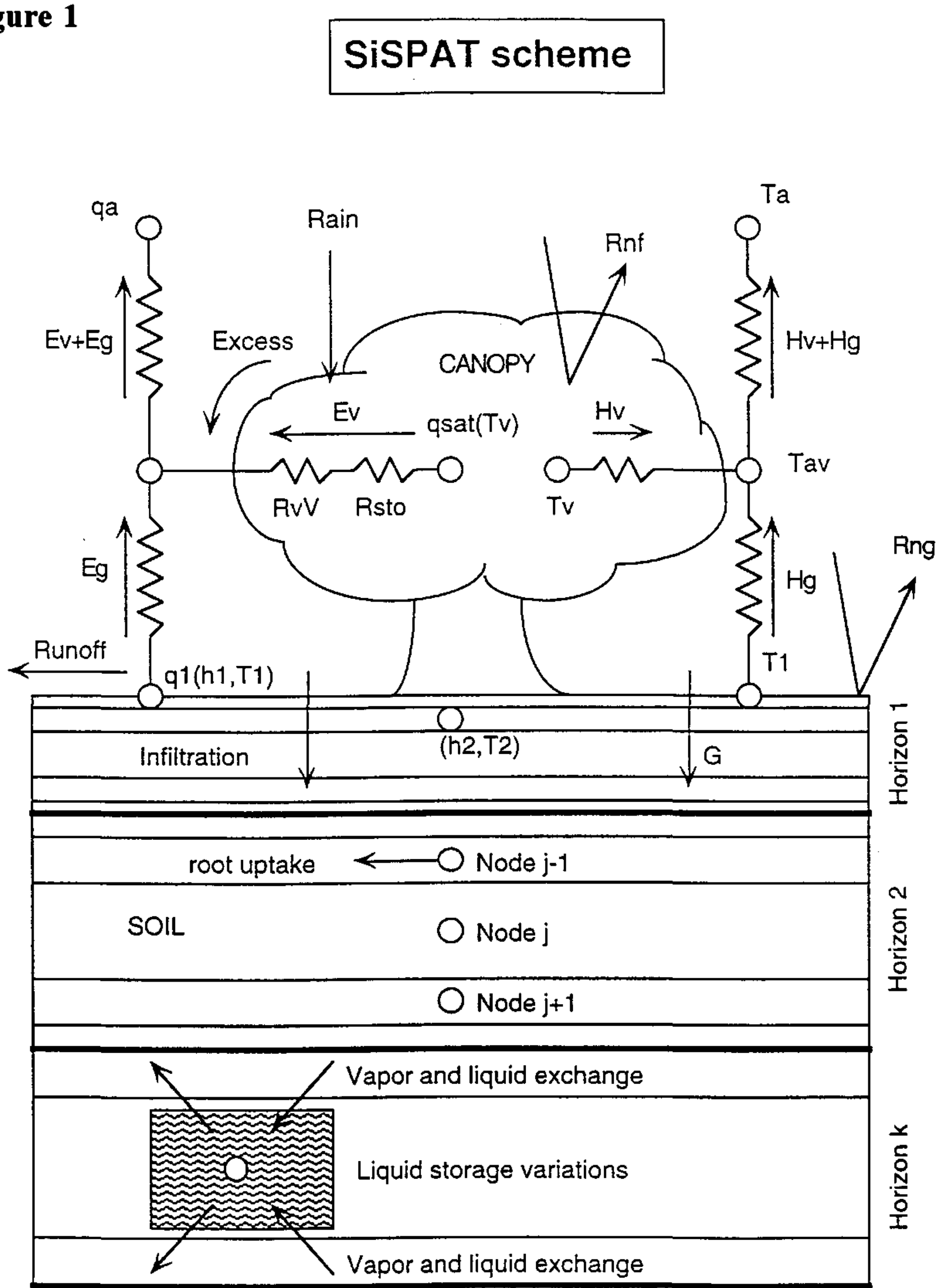


$$\begin{cases} C_h \dfrac{\partial h}{\partial t} = \dfrac{\partial}{\partial z}\left(D_{mh}\dfrac{\partial h}{\partial z} + D_{mT}\dfrac{\partial T}{\partial z} - K \right) - S \\ C_T \dfrac{\partial T}{\partial t} = \dfrac{\partial}{\partial z}\left(D_{ch}\dfrac{\partial h}{\partial z} + D_{cT}\dfrac{\partial T}{\partial z} \right) \end{cases}$$

Figure 2

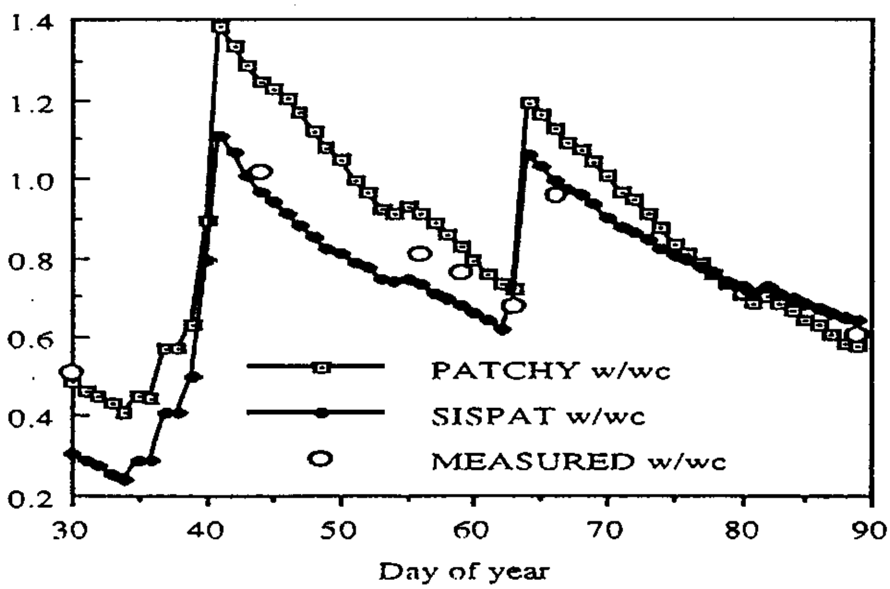


Figure 3

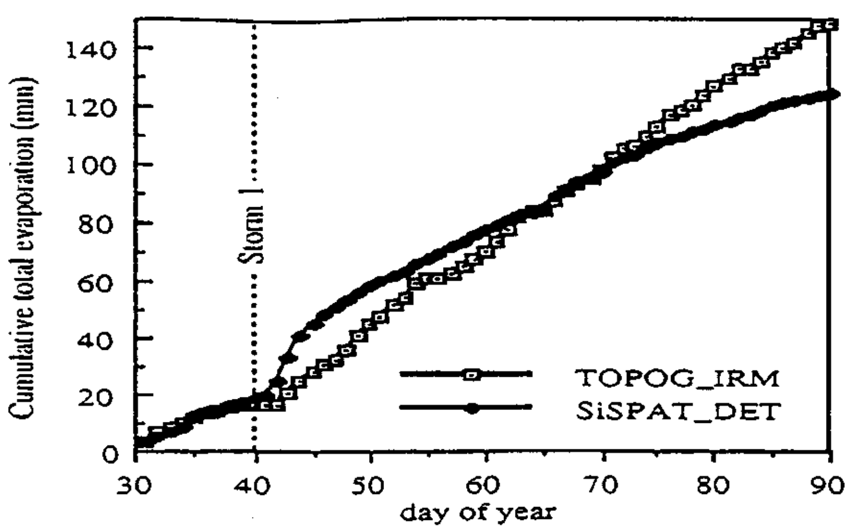
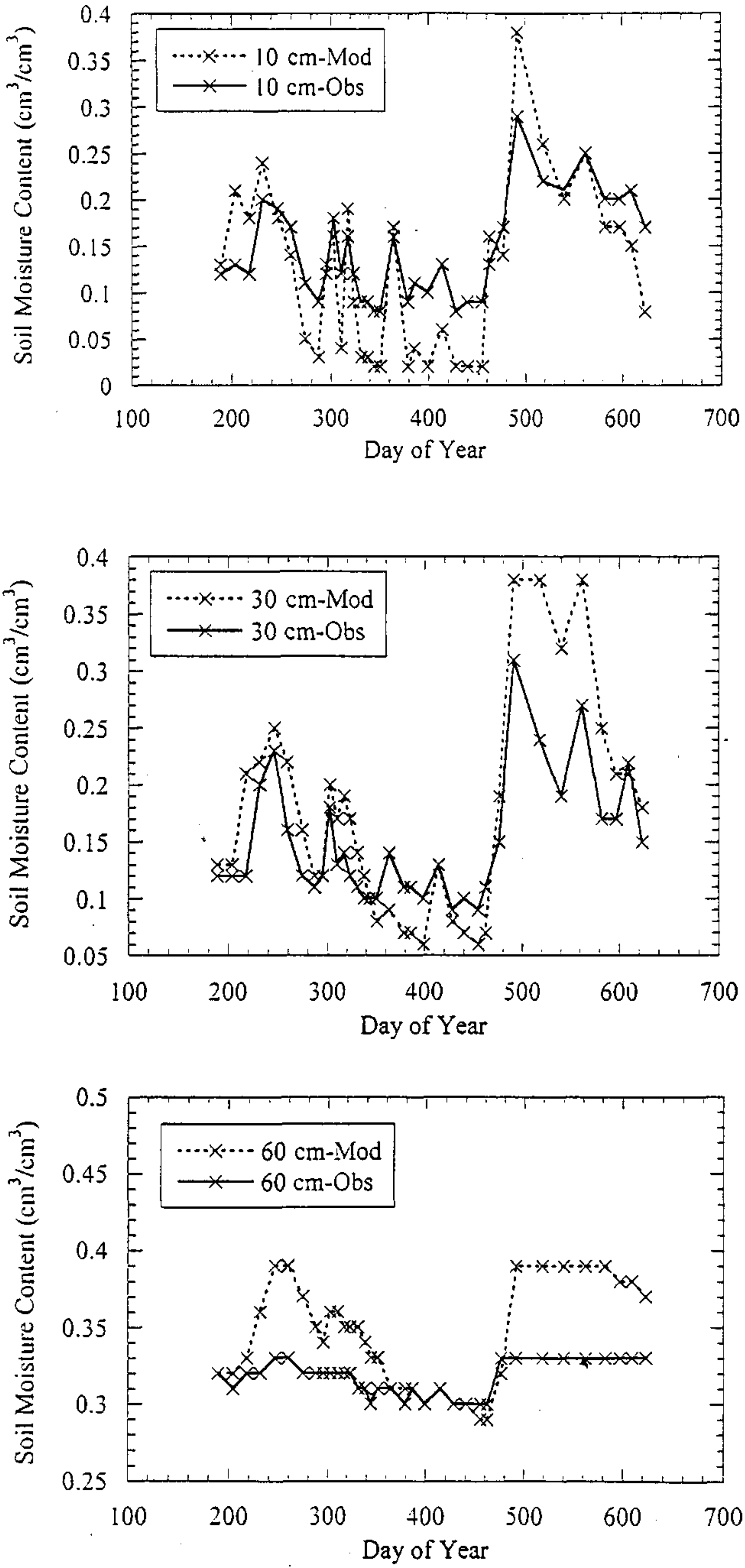
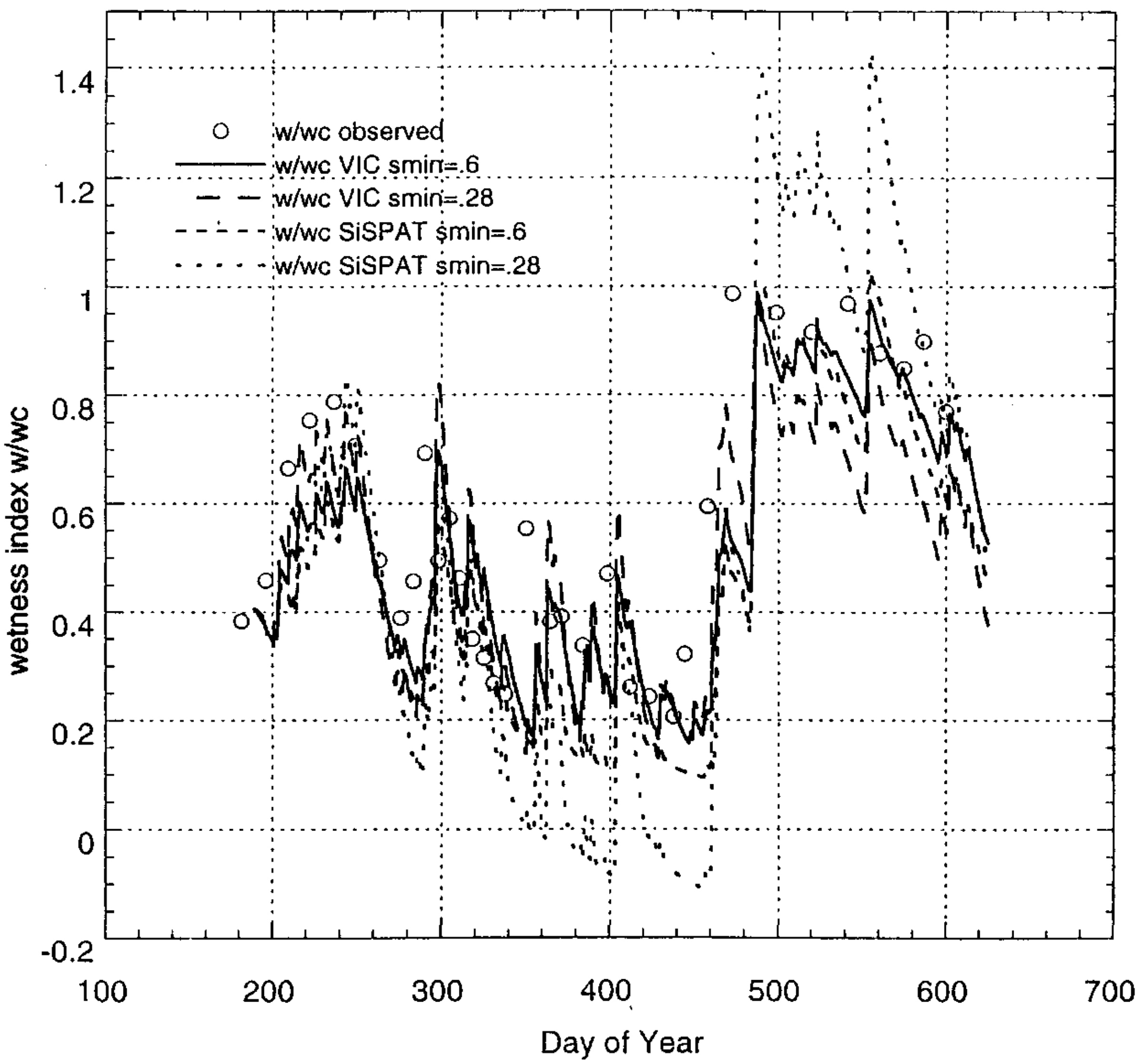


Figure 4



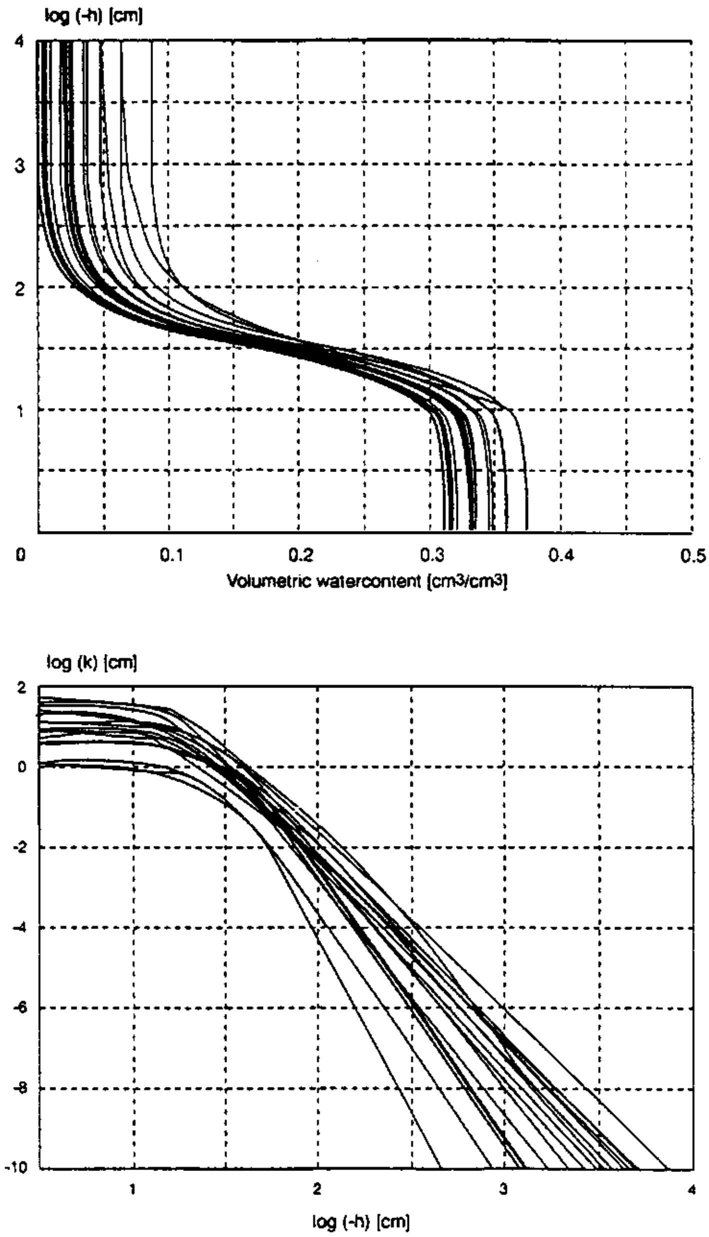
10 cm-Mod
10 cm-Obs
Soil Moisture Content (cm^3/cm^3)
Day of Year
30 cm-Mod
30 cm-Obs
Soil Moisture Content (cm^3/cm^3)
Day of Year
60 cm-Mod
60 cm-Obs
Soil Moisture Content (cm^3/cm^3)
Day of Year

Figure 5



1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
100
200
300
400
500
600
700
wetness index w/wc
Day of Year
w/wc observed
w/wc VIC smin=.6
w/wc VIC smin=.28
w/wc SiSPAT smin=.6
w/wc SiSPAT smin=.28

Figure 6a



log (-h) [cm]
4
3
2
1
0
0.1
0.2
0.3
0.4
0.5
Volumetric watercontent [cm3/cm3]
log (k) [cm]
2
0
-2
-4
-6
-8
-10
1
2
3
4
log (-h) [cm]

Figure 6b

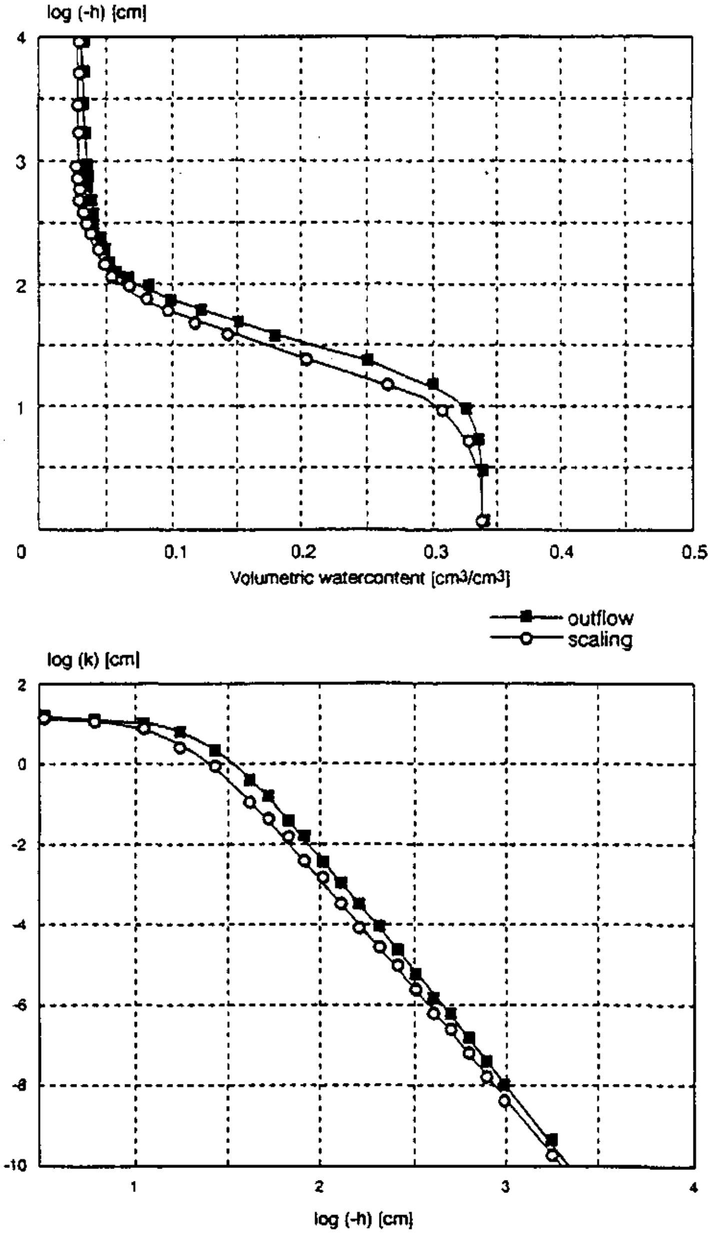
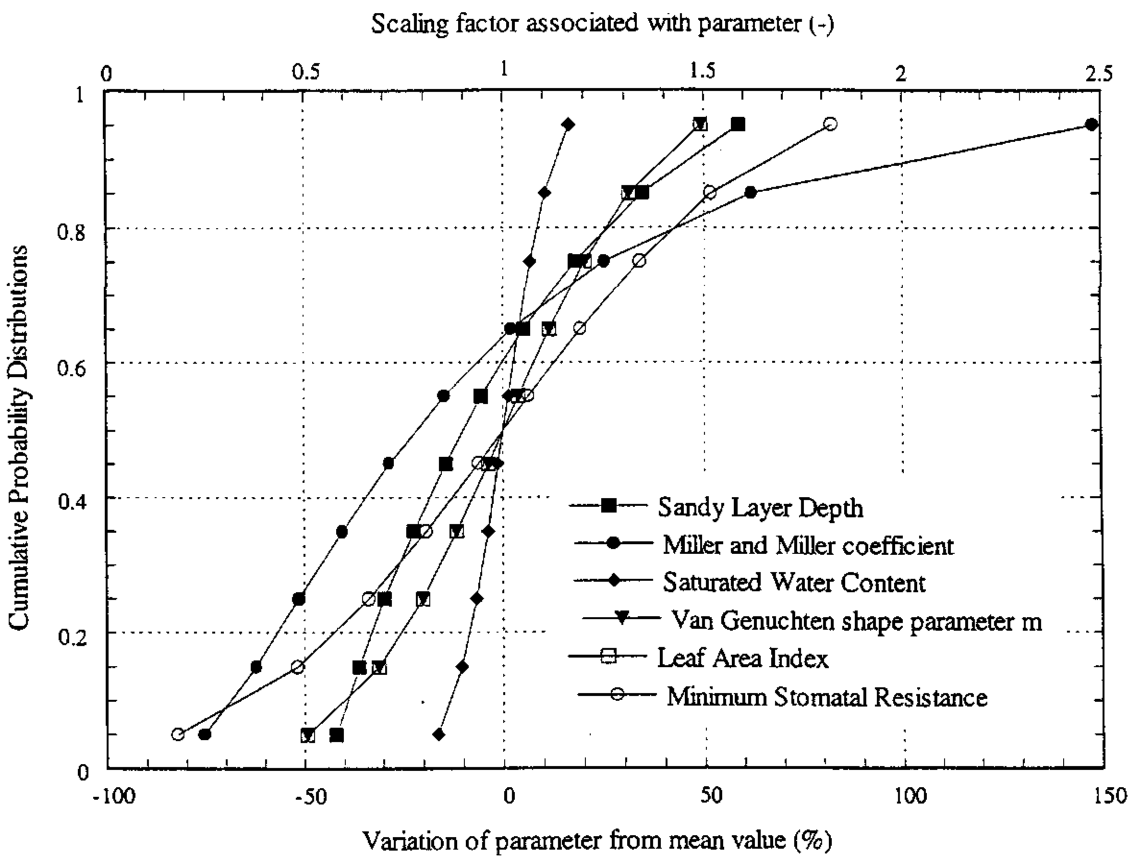

log (-h) [cm]
4
3
2
1
0
0.1
0.2
0.3
0.4
0.5
Volumetric watercontent [cm3/cm3]
outflow
scaling
log (k) [cm]
2
0
-2
-4
-6
-8
-10
1
2
3
4
log (-h) [cm]

Figure 7



Scaling factor associated with parameter (-)
0
0.5
1
1.5
2
2.5
1
0.8
0.6
0.4
0.2
0
Cumulative Probability Distributions
Sandy Layer Depth
Miller and Miller coefficient
Saturated Water Content
Van Genuchten shape parameter m
Leaf Area Index
Minimum Stomatal Resistance
-100
-50
0
50
100
150
Variation of parameter from mean value (%)

Figure 8

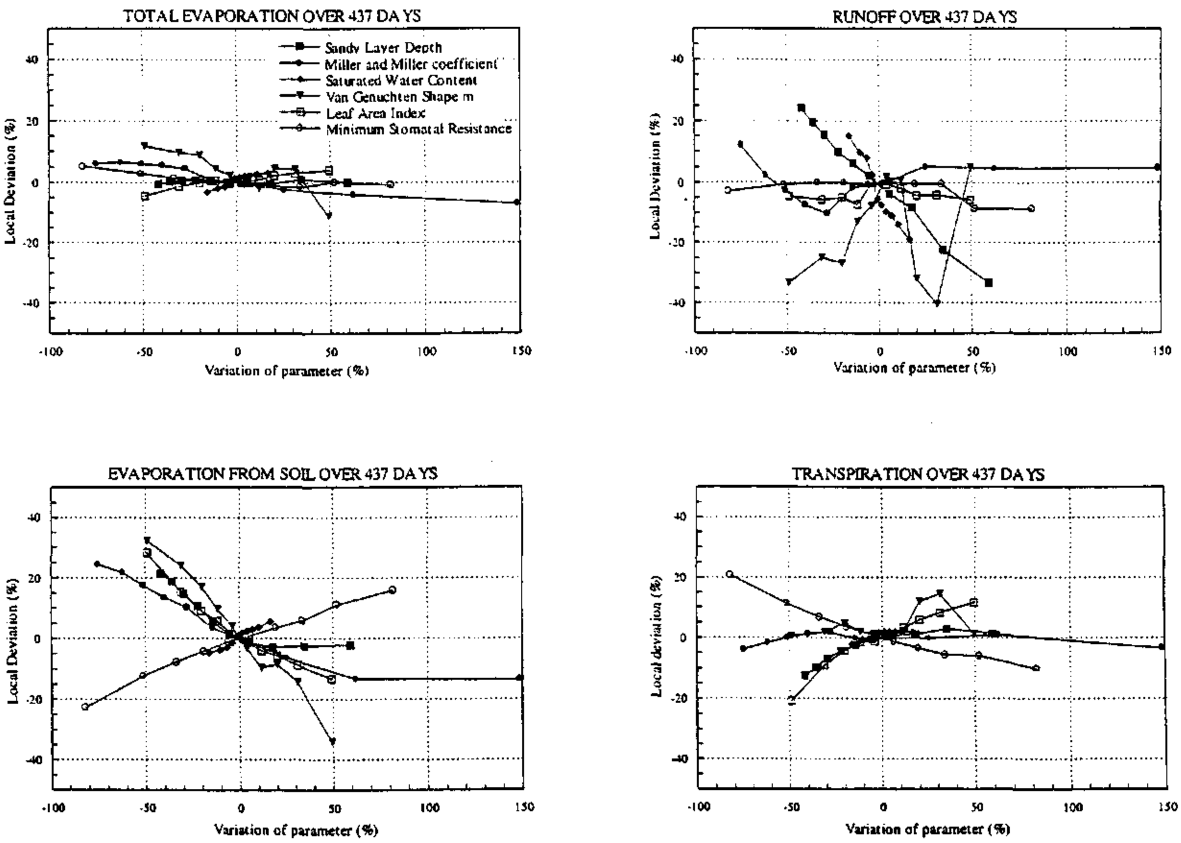

TOTAL EVAPORATION OVER 437 DAYS
Sandy Layer Depth
Miller and Miller coefficient
Saturated Water Content
Van Genuchten Shape m
Leaf Area Index
Minimum Stomatal Resistance
Local Deviation (%)
Variation of parameter (%)
RUNOFF OVER 437 DAYS
Local Deviation (%)
Variation of parameter (%)
EVAPORATION FROM SOIL OVER 437 DAYS
Local Deviation (%)
Variation of parameter (%)
TRANSPIRATION OVER 437 DAYS
Local deviation (%)
Variation of parameter (%)

Figure 9

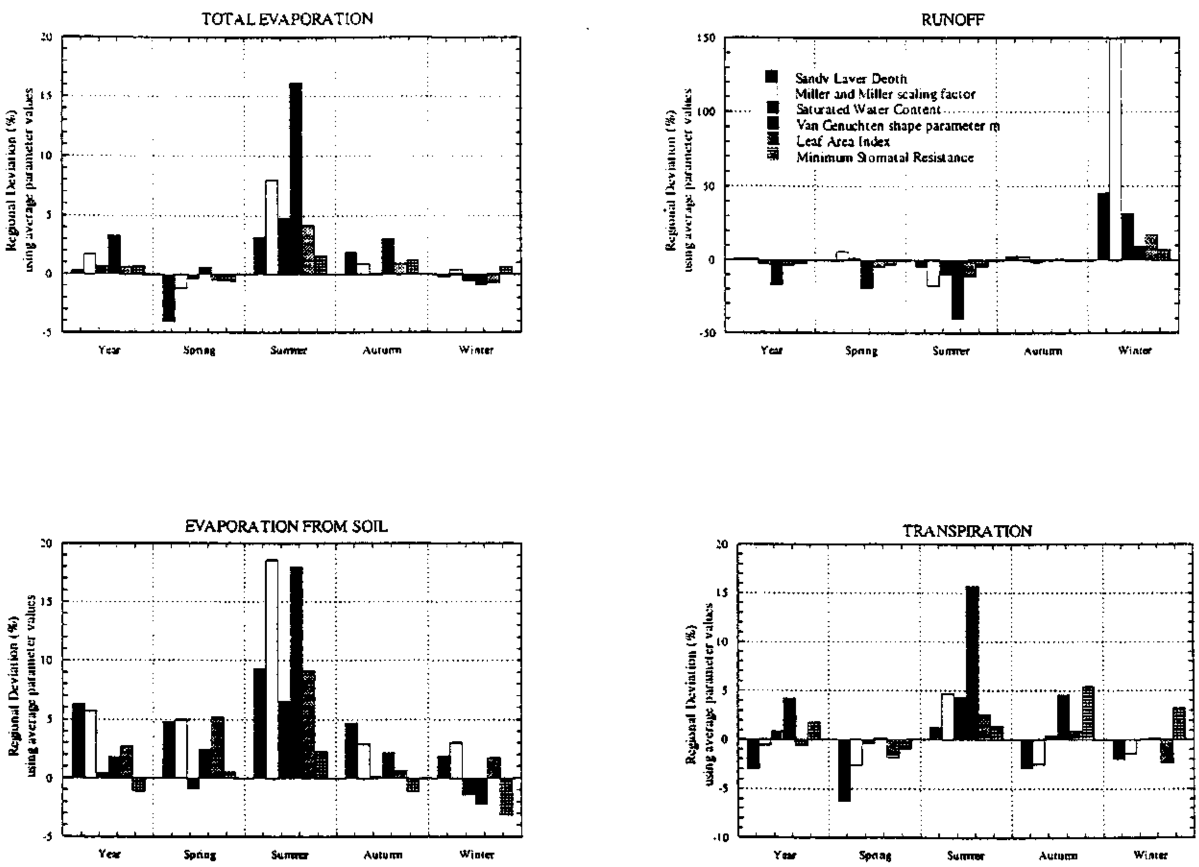
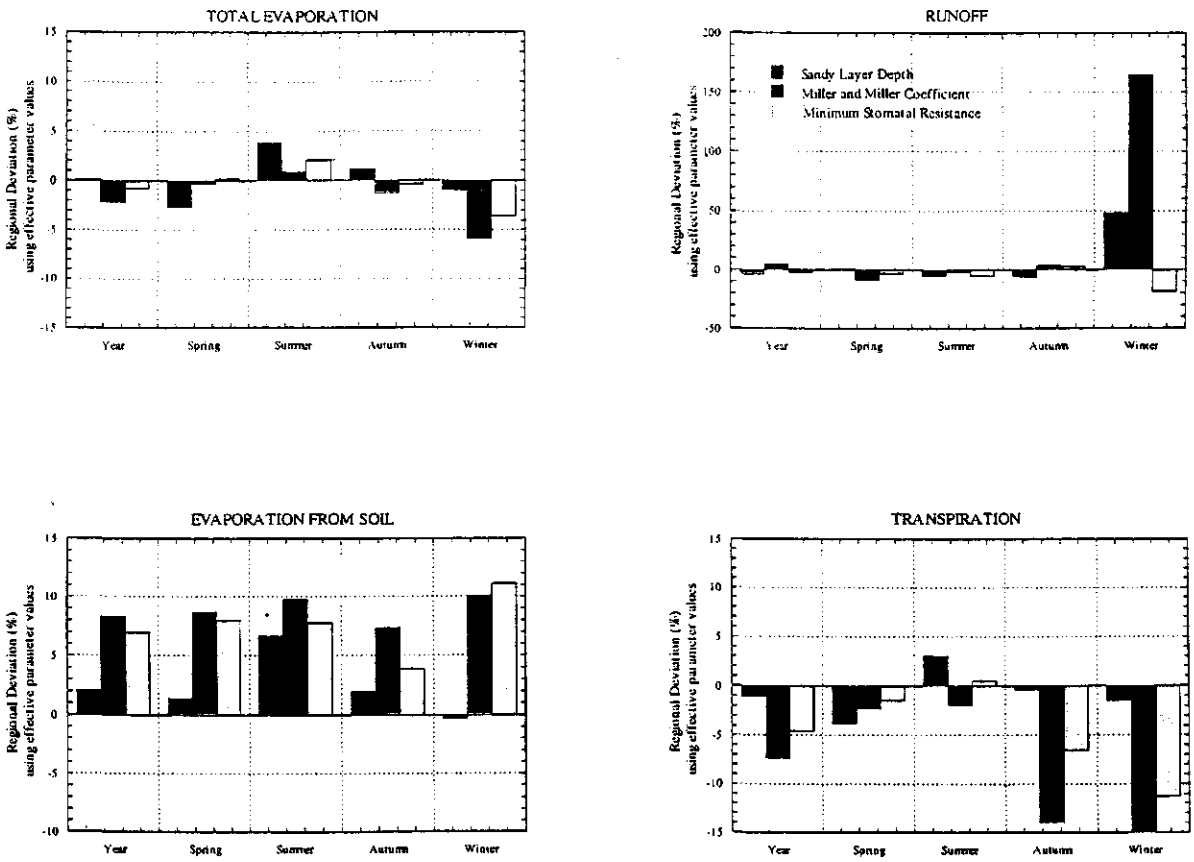
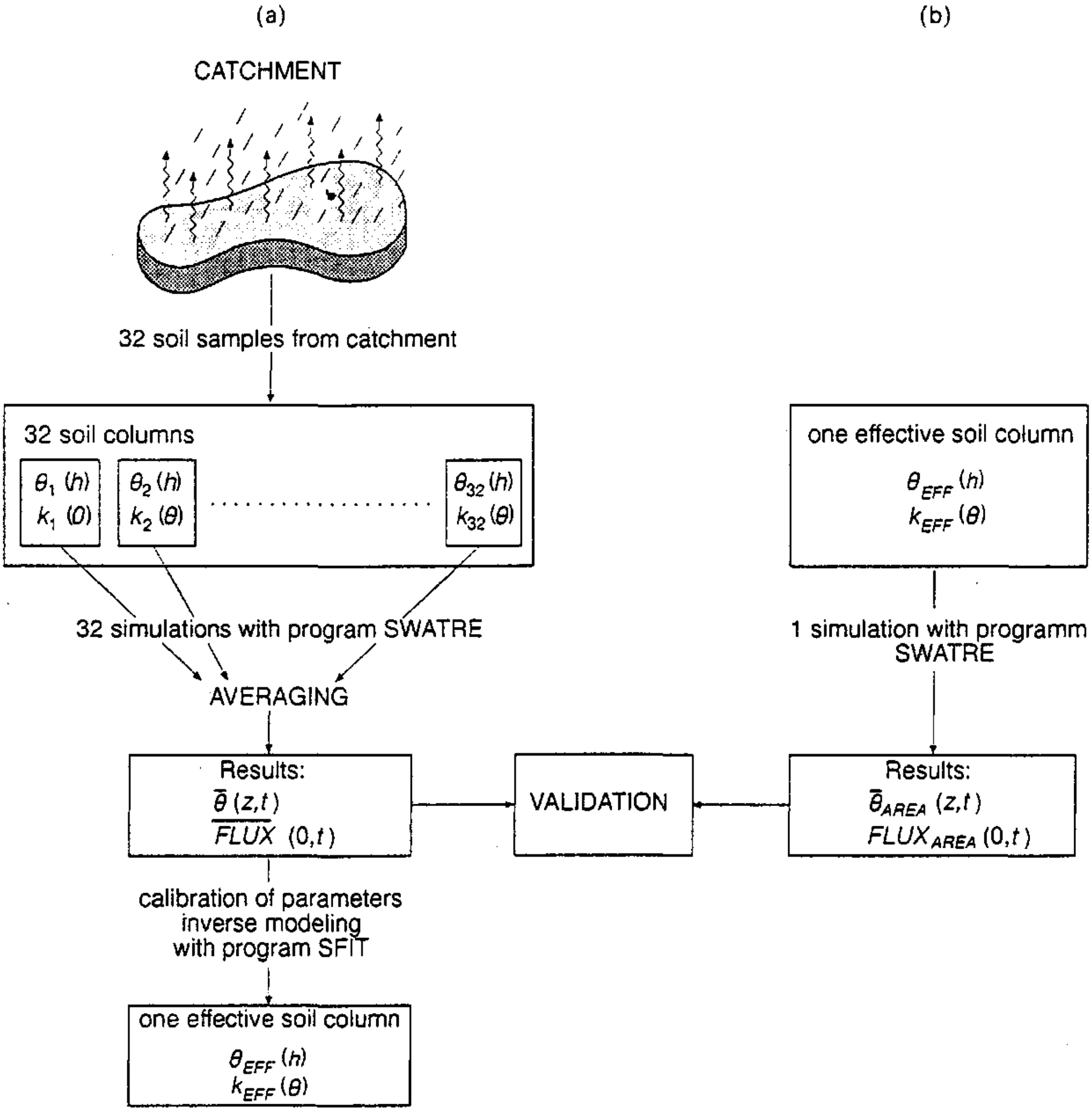

TOTAL EVAPORATION
RUNOFF
EVAPORATION FROM SOIL
TRANSPIRATION
Sandy Layer Depth
Miller and Miller scaling factor
Saturated Water Content
Van Genuchten shape parameter m
Leaf Area Index
Minimum Stomatal Resistance
Regional Deviation (%)
using average parameter values
Year
Spring
Summer
Autumn
Winter

Figure 10



TOTAL EVAPORATION
RUNOFF
EVAPORATION FROM SOIL
TRANSPIRATION
Regional Deviation (%) using effective parameter values
Sandy Layer Depth
Miller and Miller Coefficient
Minimum Stomatal Resistance
Year
Spring
Summer
Autumn
Winter

Figure 11



(a)
(b)
CATCHMENT
32 soil samples from catchment
32 soil columns
θ_1 (h)
k_1 (0)
θ_2 (h)
k_2 (θ)
θ_{32} (h)
k_{32} (θ)
one effective soil column
θ_{EFF} (h)
k_{EFF} (θ)
32 simulations with program SWATRE
1 simulation with programm SWATRE
AVERAGING
Results:
$\bar{\theta}$ (z,t)
$\overline{FLUX}$ (0,t)
VALIDATION
Results:
$\bar{\theta}_{AREA}$ (z,t)
$FLUX_{AREA}$ (0,t)
calibration of parameters
inverse modeling
with program SFIT
one effective soil column
θ_{EFF} (h)
k_{EFF} (θ)

Figure 12

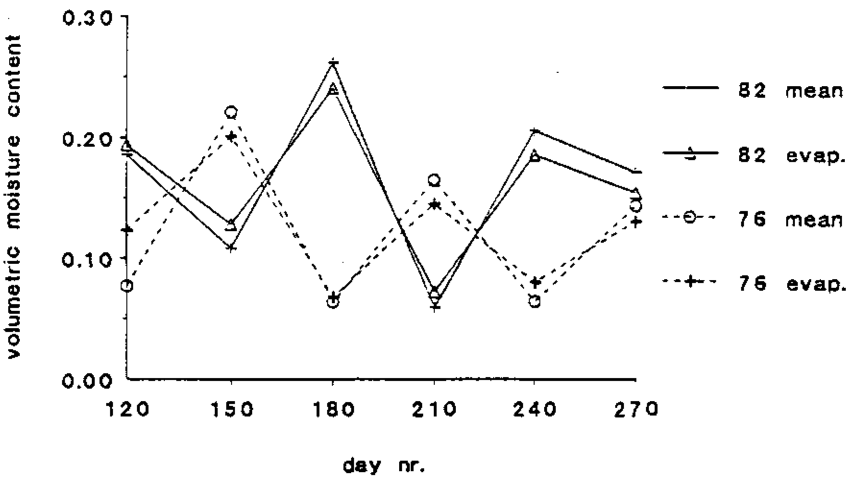


Figure 13

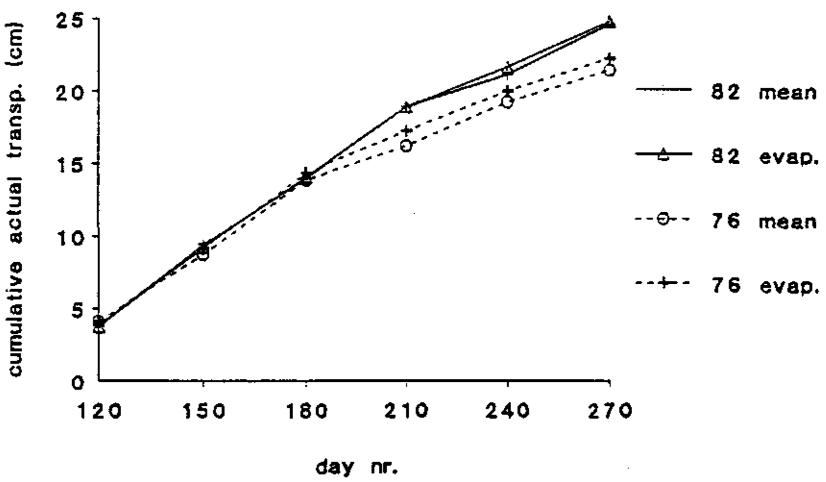


Figure 14

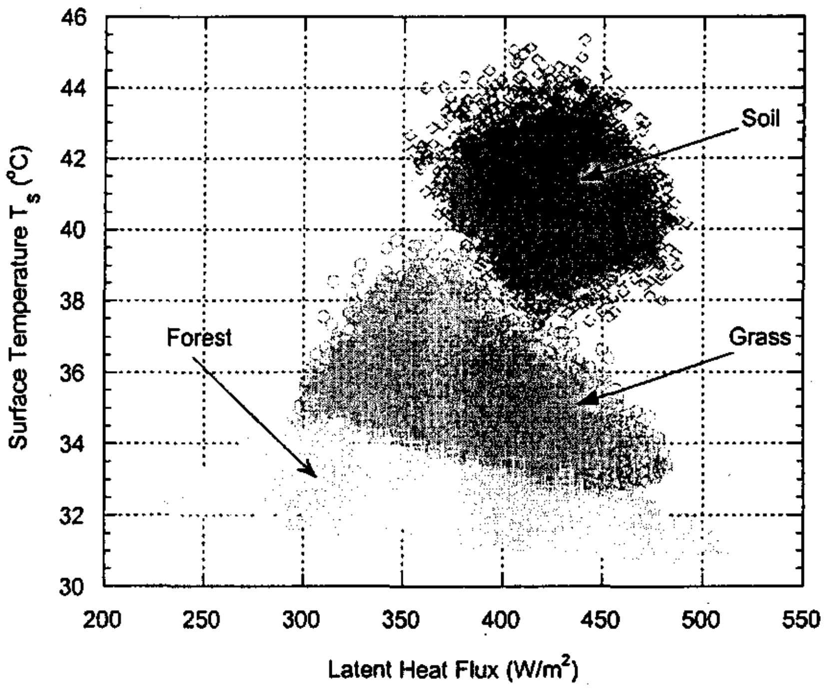
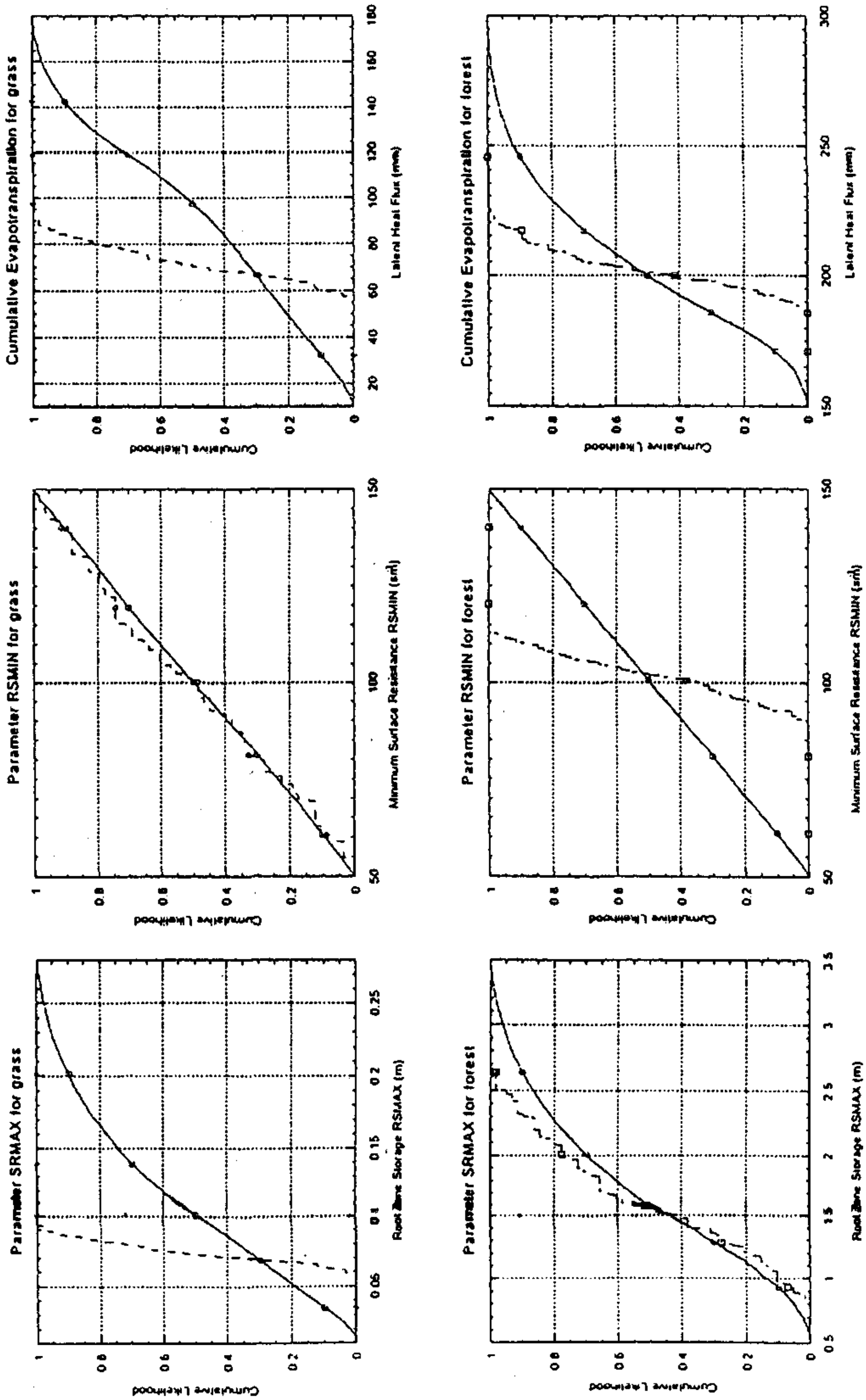

46
44
42
40
38
36
34
32
30
Surface Temperature T_s (°C)
200
250
300
350
400
450
500
550
Latent Heat Flux (W/m^2)
Soil
Grass
Forest

Figure 15



Cumulative Evapotranspiration for grass
Latent Heat Flux (mm)
Parameter RSMIN for grass
Minimum Surface Resistance RSMIN (s/m)
Parameter SRMAX for grass
Root Zone Storage RSMAX (m)
Cumulative Evapotranspiration for forest
Latent Heat Flux (mm)
Parameter RSMIN for forest
Minimum Surface Resistance RSMIN (s/m)
Parameter SRMAX for forest
Root Zone Storage RSMAX (m)
Cumulative Likelihood

Figure 16

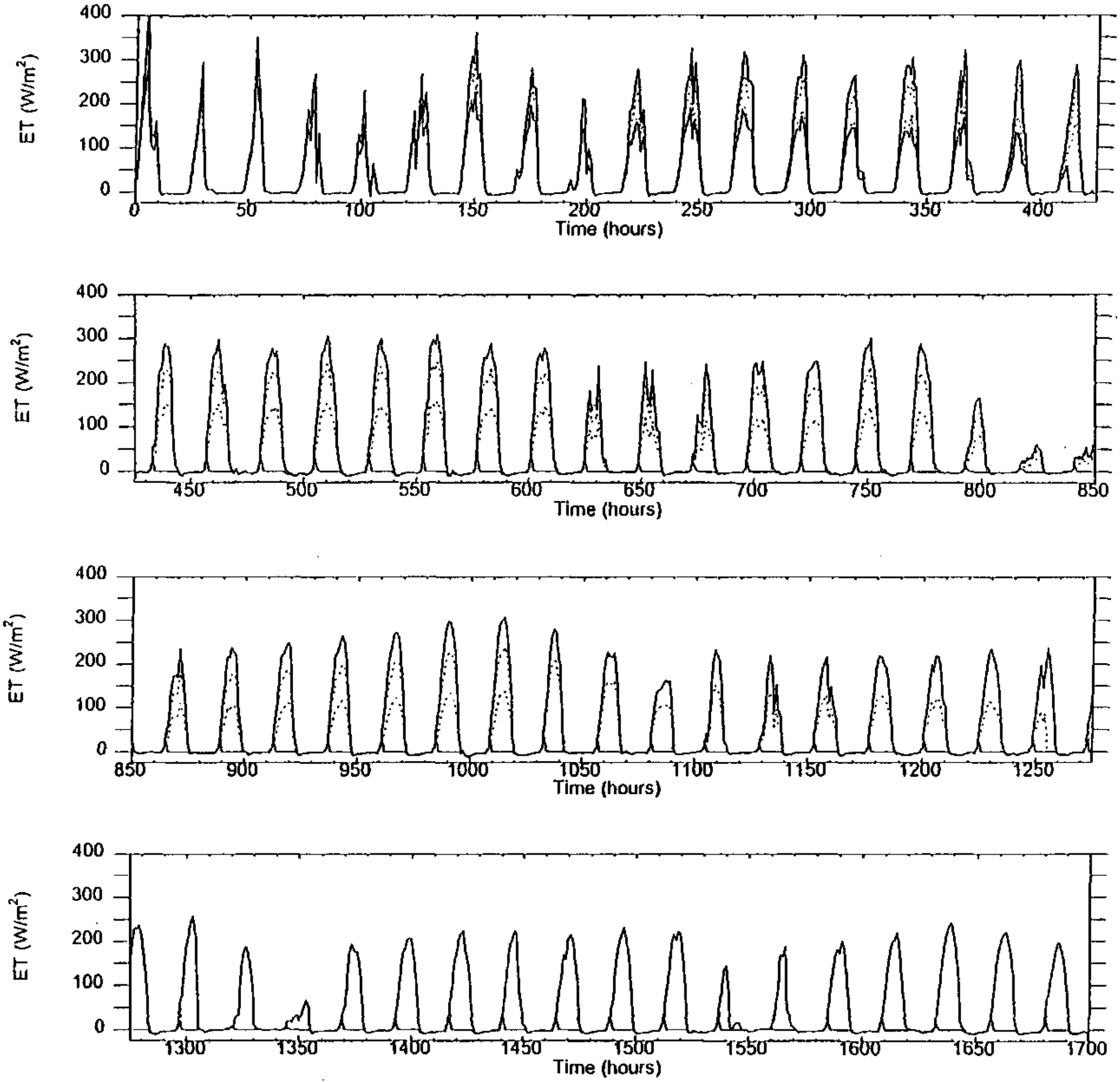

400
300
200
100
0
ET (W/m^2)
0
50
100
150
200
250
300
350
400
Time (hours)
450
500
550
600
650
700
750
800
850
Time (hours)
850
900
950
1000
1050
1100
1150
1200
1250
Time (hours)
1300
1350
1400
1450
1500
1550
1600
1650
1700
Time (hours)

Table 1

(mm)	TOPOG—IRM	SiSPAT—DET
Rain	218	218
Soil evaporation	126	90
Transpiration	23	33
Runoff (observed runoff: 21)	9	23
Deep drainage	1	29
Storage	66	43

Table 2

Scaled quantity	Symbol	Analytical statistical law	σ
Sandy layer thickness	z_{sand}	Xinanjiang (see text)	0.34
Miller and Miller coefficient	α	Log-normal	0.82
Saturated water content	θ_{sat}	Normal	0.11
Van Genuchten shape parameter	m	Normal	0.34
Leaf Area Index (114 points)	LAI	Normal	0.3
Minimum stomatal resistance	R_{stmin}	Normal	0.5

Table 3

Varied Parameters		Parameter Ranges		
		Soil	*Grass*	*Forest*
h_c	canopy height (m)	0	0.1 – 1	5 – 12
β	% net radiation returned as ground heat flux	←	0.15 – 0.25	→
RSMIN	minimum surface resistance (sm^{-1})	←	50 – 150	→
RSMAX	maximum surface resistance (sm^{-1})	←	300 – 1000	→
$\ln(z_0/z_h)$	ratio of z_0 for momentum & heat flux	←	1 – 3	→
SRMAX	root zone storage (m)	0.01 – 0.1	← $0.1 h_c - 0.3 h_c$ →	
z_0	roughness length for momentum flux	< 0.0005	← $\gamma (h_c - d)$ →	
D	zero displacement height	0	← $0.6 h_c - 0.7 h_c$ →	
γ	coefficient used in z_0 calculation	-	← 0.2 – 0.4 →	