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Geoderma 134 (2006) 253 – 266
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Information content and complexity of simulated soil water fluxes

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Available online 19 April 2006

Abstract

The accuracy-based performance measures may not suffice to discriminate among soil water flow models. The objective of this work was to attempt using information theory measures to discriminate between different models for the same site. The Richards equation-based model HYDRUS-1D and a water budget-type model MWBUS were used to simulate one-year long observations of soil water contents and infiltration fluxes at various depths in a 1-m deep loamy Eutric Regosol in Bekkevoort, Belgium. We used the (a) metric entropy and (b) the mean information gain as information content measures, and (c) the effective measure complexity and (d) the fluctuation complexity as complexity measures. To compute the information content and complexity measures, time series of fluxes were encoded with the binary alphabet; fluxes greater (less) than the median value were encoded with one (zero). Fifty Monte Carlo simulation runs were performed with both models using hydraulic properties measured along a trench. The two models had the similar accuracy of water flux simulations. Precipitation input data demonstrated a moderate complexity and relatively high information content. Model outputs showed distinct differences in their relationships between complexity and information content. Overall, more complex simulated soil flux time series were obtained with the HYDRUS-1D model that was perceived to be conceptually more complex than the WMBUS model. An increase in the complexity of water flux time series occurred in parallel with the decrease in the information content. Using both complexity and information content measures allowed us to discriminate between the soil water models that gave the same accuracy of soil water flux estimates.
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1. Introduction

The search for discriminating between soil water flow models has intensified as the number of such models has been steadily growing. Practical problems of soil water flow are rarely tackled with more than one model. Therefore, if many models are available, it is desirable to have a measure of their performance at a specific site to justify a choice in favor of one of the models.

Residuals, i.e. differences between simulated and measured values, are commonly used to evaluate performance of models. Most of commonly used performance measures such as the root-mean square error, the lack-of-fit root mean square error (Whitmore, 1991), Williams–Kloot test (Pachepsky et al., 2000), modeling efficiency (Loague and Green, 1991), use the statistics or probability distribution functions of the set of residuals.

Residual-based performance measures quite often cannot discriminate models. Residuals quantify the model accuracy, and one can conclude that the accuracy

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0016-7061/$ - see front matter. Published by Elsevier B.V.
doi:10.1016/j.geoderma.2006.03.003

of models is similar if some statistics of residuals are similar. However, the differences between models should not be viewed only in terms of the model accuracy. The accuracy reflects only a specific instance of model performance with respect to a specific data set used for testing and/or calibration. Once calibrated, soil water flow models are usually used in Monte Carlo-type simulations with multiple scenarios of boundary conditions, initial conditions, and possibly soil and plant properties. Therefore, other performance measures should be sought that reveal the differences between models under scenarios that have not been observed.

The information theory was successfully used for the model discrimination purpose in cases when the main difference between models was the difference in the number of parameters and parameters were qualitatively similar, like regression coefficients or hydraulic conductivities of different geological bodies in groundwater transport modeling. Akaike criterion (Akaike, 1973) and its versions (Bozdogan, 1987; Hurvich and Tsai, 1989) discriminate models by computing the relative entropy, or Kullback–Leibler "distance," which represents the information loss when a model is used to approximate data. Those criteria introduce information theory measures to gauge a model performance with respect to a given dataset. But they do not reveal the differences between model behavior with input scenarios different from the ones in observations.

Usually the differences between models of flow and transport in soils are discussed in terms of model structural complexity and detail. The model complexity can be evaluated in terms of the number of processes being considered explicitly, process descriptions, spatial and temporal discretization/scale, number of parameters, and speed of computations (Neuman et al., 2003). The numbers characterizing those model features are hardly compatible, and their relative significance is unknown. For example, the total number of parameters is not a comprehensive index of model complexity, because the sensitivity of model outputs to some parameters can be relatively low, and may depend on the scenario.

Unlike model structures, model outputs are compatible, because soil water flow models under comparison should generate time series of water fluxes or water contents for the same depths. Given one cannot discriminate models based on complexity of models structures, is it possible to discriminate models based on the complexity of model output? Some measures of time series complexity are needed to do that. The information theory has been used to propose several such measures (Wackerbauer et al., 1994). Lange (1999a,b) suggested using information-related measures to discriminate between measured time series. He made the distinction between the information content, or the randomness, of data on one hand, and their complexity on the other. By the latter he meant a measure which vanishes or is very small both for constant or periodic sequences and for completely random data, as both types are easy to describe. The complexity measures should show high values for time series not amenable to an easy description involving only a few parameters. This (admittedly intuitive) distinction is illustrated in Fig. 1. Complexity and information content of daily runoff and precipitation are presented in Fig. 2 for several catchments in Germany and New Hampshire (Lange, 1999a,b). Runoff from the natural catchments operates at high complexities and

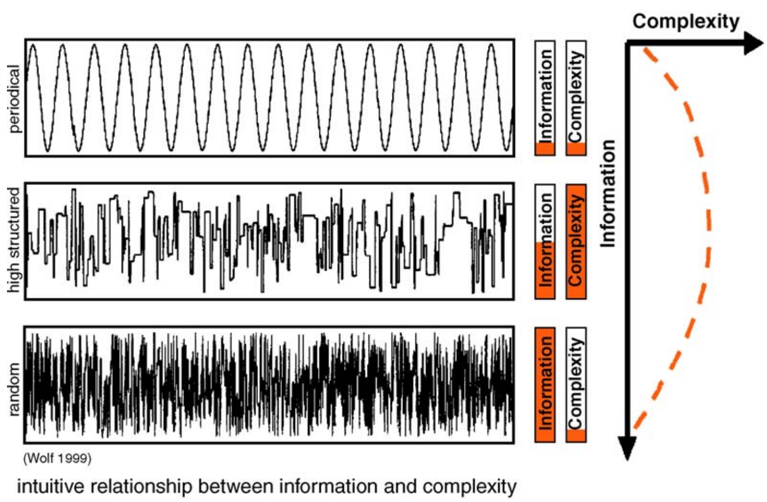

Fig. 1. Complexity and randomness for the sine function, the highly structured Bernoulli process with the probability of repetition 83%, and the random process with the uniform distribution (Wolf, 1999).

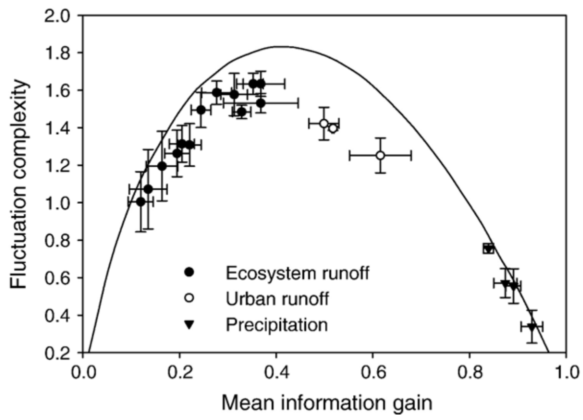

Fig. 2. Randomness, quantified with the mean information gain, and complexity, quantified with the fluctuation complexity, in daily time series of precipitation and runoff from ecosystems and urban storm drain systems (Lange, 1999a).

intermediate randomness, urban (channeled) systems have much more randomness. Precipitation is characterized by extremely high randomness and low complexity. Data in Fig. 2 show the potential of information theory measures to discriminate water flux time series generated in the system of different complexity. Recently Selle and Huwe (2004) proposed to discriminate soil water models using information theory measures.

The objective of this work was to evaluate the effectiveness of the information theory measures to discriminate between different models using simulated time series of soil water fluxes for the same site. We wanted to see whether and how the perceived differences between model structures manifest themselves in differences in information content and complexity of the simulated time series of soil water fluxes.

2. Theory

This section introduces information theory-based measures of information content and complexity. First, such measures are defined for systems having a finite number of states. Then a method is described to represent a time series with a system with the finite number of states. Such system appears to be a binary string. Finally, several information theory variables are listed that measure both randomness and complexity of binary strings.

2.1. Information content and complexity in systems with a finite number of states

Consider a system that has N possible different states. Let p_i be the probability of the ith state, $p_{i\to j}$ be the probability of the transition from the state "i" to the state "j" provided state "i" was reached, and p_{ij} be the probability of that the transition from state "i" to state "j" actually occurs. Those probabilities are related: $p_{ij}=p_i p_{i\to j}$.

Knowledge of state and transition probability permits computing several information variables (Bates and Shepard, 1993). Shannon (1948) defined the information I_i specifying the state "i" of a system as

$$I_i = \log_2\left(\frac{1}{p_i}\right) \tag{1}$$

The average value of the information about the system is its Shannon's entropy:

$$H = \sum_{i=1}^{N} p_i I_i = -\sum_{i=1}^{N} p_i \log_2 p_i \tag{2}$$

It has the maximum value of log(N) when all states are equally probable and $p_i=1/N$, $i=1, 2, 3,\dots N$; H is measured in bits.

The information gain G_{ij} associated with transition from the state "i" to state "j" is

$$G_{ij} = \log_2\left(\frac{1}{p_{i\to j}}\right) \tag{3}$$

Similarly, the information loss L_{ij} is defined as

$$L_{ij} = \log_2\left(\frac{1}{p_{j\to i}}\right) \tag{4}$$

where the state "j" occurs after the state "i". The net information gain is the difference between the information gain and loss:

$$\Gamma_{ij} = G_{ij} - L_{ij} = \log(p_{j\to i}/p_{i\to j}) = \log_2\frac{p_i}{p_j} \tag{5}$$

The average value of Γ_{ij} over all possible transitions is zero. The mean square deviation σ_Γ^2 of values Γ_{ij}

$$\sigma_\Gamma^2 = \sum_{i,j}^{N} p_{ij}\left(\log_2\frac{p_i}{p_j}\right)^2 \tag{6}$$

is not zero. This value has been termed fluctuation complexity (Bates and Shepard, 1993). It captures the fluctuations in the system occurring as it performs transitions from state to another. The fluctuation complexity thus measures the spread between information that a system may have in its consecutive states. The fluctuation complexity is zero in systems with maximum entropy where all states are equiprobable (all $p_i=1/N$). The fluctuation complexity approaches zero in systems with the entropy approaching zero that have only one highly probable state.

2.2. Representing a time series with a system with the finite number of states

To represent a time series with a system with the finite number of states, the time series is encoded as a symbol string. Lange (1999a) suggested the binary encoding in which each observation in the time series is encoded as zero or one. Specifically, all values larger than the median value of all observations are encoded as one, and all values less than the median value of all observations are encoded as zero. Then the word length L is defined to group consecutive symbols together. A word of L consecutive symbols (zeros and ones) is a state of the system of interest. This system has the finite number 2^L of possible states. An example of such encoding is shown in Fig. 3. If one considers three-symbol words ($L=3$), then all possible words are 000, 001, 010, 011, 100, 101, 110, 111, total of $2^3=8$ words.

The transition in the string is the shift by one symbol. For example, if the string is “00110” and the word length is three symbols, then the first word “001” transits to the second word “011”, and the second word “011” transits to the third word “110”. The first and the second word in transitions overlap by $L-1$ symbol which are the last $L-1$ symbol of the first word and the first $L-1$ symbol for the second word.

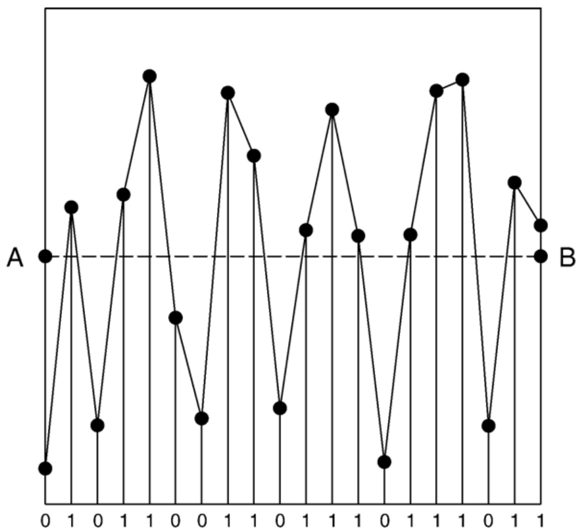

Fig. 3. Example of the binary encoding of a time series. The line AB shows the median value of the observations in the time series.

The probabilities defined for the binary string are:

$p_{L,i}$ probability of the occurrence of the ith word,

$p_{L,ij}$ probability of the transition from the ith to the jth L-word.

$p_{L,i\to j}$ conditional probability of the occurrence of the jth word after ith word, i.e. occurrence of the jth word provided that the ith word has occurred.

2.3. Information theory measures for binary strings representing time series

The information theory offers many variables suitable to measure the information content and complexity of symbolic string sequences (Wackerbauer et al., 1994). The following variables were selected for this work.

The information content was measured with the metric entropy and mean information gain. The Shannon entropy given by Eq. (2) can be computed for words of length L as

$$H(L) = -\sum_{i=1}^{2^L} p_{L,i}\log_2 p_{L,i} \tag{7}$$

The Shannon entropy increases linearly with increasing word length. Normalization with the word length yields the notion of information independently of the word length. This measure is called metric entropy H_μ:

$$H_\mu = H(L)/L \tag{8}$$

The metric entropy vanishes for constant sequences, increases monotonically when the sequence's disorder raises and reaches its maximum at 1 for uniformly distributed random sequences.

The knowledge of a symbol that follows a word contributes to the local information. This knowledge reflects the information gain G as given in Eq. (3). The average, or mean information gain is

$$H_G(L) = -\sum_{i,j=1}^{2^L} p_{L,ij}\log_2 p_{L,i\to j} \tag{9}$$

The mean information gain H_G tells how much additional information will be gained in average for the whole symbol sequence by knowing the next symbol. The effect of the knowledge of the next symbol on the information can be illustrated by the following example (Wolf, 1999). If one observes the sequence of letters “info” within this text, then the following letter will be an “r” for sure. The knowledge of this following letter does not contribute to the information. But, if we have observed the sequence "the," then it is really hard to predict the next letter. Any letter is possible. Here the knowledge of the next letter is a real gain of information.

The complexity of symbolic strings was quantified in this work using the fluctuation complexity value and the effective complexity values as defined below. The fluctuation complexity is computed for a string according to Eq. (6) as

$$\sigma_{\Gamma}^2 = \sum_{i,j}^{2^L} p_{L,ij}\left(\log_2 \frac{p_{L,i}}{p_{L,j}}\right)^2 \quad (10)$$

Wolf (1999) gives the following example of the interpretation of the fluctuation complexity. If one observes the sequence of letters "info" within this text, then the following letter will be an "r" for sure. However, if the word 'nfor' is observed, then the information gain by knowing the "r" is zero within this text, whereas the information loss of forgetting the "i" is higher, because "nfor" occurs in the words "unfortunately" and "Information" with a capital "I" (at the begin of a sentence or in headings). The more these differences of information gain and loss is fluctuating in the investigated string, the more complex is the string in the sense of the fluctuation complexity.

The effective measure complexity C_{EM} evaluates the minimum total amount of information that has to be stored at any time for an optimal prediction of the next symbol (Grassberger, 1986). This measure can approximately be computed as

$$C_{\mathrm{EM}} = \sum_{i,j=1}^{2^L} p_{L,ij}\log_2 \frac{p^L_{L,i\rightarrow j}}{p_{L,i}} \quad (11)$$

The length of words L is arbitrary in theory but is limited in applications because all measures of information and complexity are dependent on probability distributions of words and transitions in symbolic strings, and the probabilities have to be estimated as the relative frequencies. The availability of data limits the ability to estimate the probabilities by relative frequencies. Wolf (1999) suggested to estimate the word length for the worst-case scenario of uniformly distributed random sequences. The theoretical value of the measures in this case is known. Thus, a condition of tolerance for the deviation (relative precision) of the expected value compared to the theoretical value can be found. The Table 1 presents Wolf's requirements to the length of the binary string for 3 and 4 symbol words if a 5% relative error is acceptable.

Table 1
Total numbers of symbols in binary strings to provide 5% or better accuracy in information and complexity measure estimations

Information theory measure	Two-symbol words	Three-symbol words	Four-symbol words
Metric entropy	24	38	62
Mean information gain	63	124	246
Fluctuation complexity	146	262	491
Effective measure complexity	79	256	723

All information theory measures were computed in this work using the SYMDYN software available at the Internet at http://www.dr-frank-wolf.de/diss/dissen.htm. The length of words permitted by the volume of our data was two.

3. Experimental data

The experimental setup has been described earlier by Jacques et al. (2002). In brief, the experimental field was located at Bekkevoort, Belgium, at the bottom of a gentle slope and was covered with a meadow. The soil was classified as Eutric Regosol (FAO, 1975). Typically the top 1 m includes three soil horizons: an Ap horizon between 0 and 25 cm, a C1 horizon between 25 and 55 cm, and a C2 horizon between 55 and 100 cm. A trench, 1.2 m deep and 8 m long, was dug at the field site. A dye study revealed the occurrence of many macropores throughout the soil profile (Vanderborght et al., 2000). The grass cover was removed from the experimental area. A plastic sheet covered the side of the trench where equipment was installed. Volumetric water content was measured with TDR. Sixty TDR probes (two rods, 25 cm long, 0.5 cm rod diameter, 2.5 cm rod spacing) were installed along the trench at 12 locations with 50 cm spacing at 5 depths (15, 35, 55, 75, and 95 cm deep). The insertion point of the first TDR-probe was at 10 cm from the trench reference end. The probe locations on the trench wall, soil horizons observed on the wall, and soil texture are shown in Fig. 4. Soil texture was loam at 15, 35, and 55 cm sampling depths, and silty loam at 75 and 95 cm depths.

After all devices were installed, the trench was filled. A thin layer of gravel (1 to 2 cm) was evenly distributed on the study area: (i) to decrease the erosive effect of the rain impact on the bare soil surface, (ii) to minimize the evaporation from the soil surface, and (iii) to decrease the growth of weed on the experimental plot. Weeds were regularly removed from the site during the summer. Passive capillary samplers (PCAPS) were

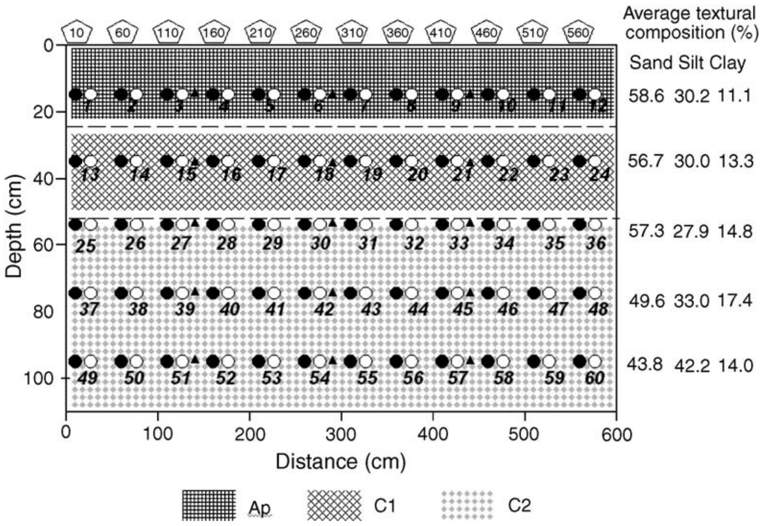

Fig. 4. Locations and numbering of TDR-probes (●), tensiometers (○) and temperature probes (□). Patterned rectangles show Ap, C1 and C2 horizons. Dashed lines show the average position of the horizon boundaries. Average values of clay, silt, and sand content are given for the probe installation depths. The numbers in pentagons show the numbering of locations monitored by five-probe profiling.

installed at two 15 and 55 cm depths at the distance of about 5 m from the trench to measure soil water fluxes once in one to three days. Field measurements started on March 11, 1998 (day 0) and finished on March 31, 1999 (day 384).

Fig. 5 shows the hourly rainfall rates and the cumulative precipitation during the experiment. A total rainfall amount of 109 cm was recorded during the period of the experiment. The average rainfall in this region is around 80 cm. The amount of rainfall was rather exceptional since it was the largest amount of rainfall during a 65-year period recorded at an official nearby weather station (Ukkel, Brussels). In the time period of the experiment, the pluviograph in Ukkel had recorded 106 cm.

Soil water fluxes were estimated at the depth of 105 cm using daily soil water balance computations based on measured water contents, precipitation, and average evaporation estimated to be 0.86 mm day^{-1}.

4. Soil water flux simulations

4.1. Soil water flow models

A Richards equation-based model and a water budget-based model were applied to simulate soil water fluxes.

The HYDRUS-1D model (Simunek et al., 1998) is a finite element model for simulating the one-dimensional movement of water, heat, and multiple solutes in variably saturated media. The program numerically solves the Richards' equation for saturated-unsaturated water flow:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial h}{\partial z} + 1\right)\right] \qquad (12)$$

where θ is the volumetric water content, h is the matric potential, K is the hydraulic conductivity, z is the vertical axis directed upward, t is time.The van Genuchten equation (van Genuchten, 1980):

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{[1 + (\alpha|h|)^n]^m} \qquad (13)$$

and the van Genuchten–Mualem equation to compute hydraulic conductivity

$$K = K_{\text{sat}}\left(\frac{\theta - \theta_{\text{r}}}{\theta_{\text{s}} - \theta_{\text{r}}}\right)^{l}\left\{1 - \left[1 - \left(\frac{\theta - \theta_{\text{r}}}{\theta_{\text{s}} - \theta_{\text{r}}}\right)^{1/m}\right]^{m}\right\}^{2} \qquad (14)$$

are used as the constitutive relationships. In Eqs. (16) and (17), θ_{s} is the saturated water content, θ_{r} is the residual water content, K_{sat} is the saturated hydraulic conductivity, 1α, m, n, and l are empirical shape-defining parameters.

The MWBUS (*m*odel of *w*ater *b*udget of *u*nsaturated *s*oils) model has been developed to provide a simple and robust description of water flow in layered soils with the daily time step. Soil is divided in layers of thickness Δz_i, $i = 1, 2, \ldots, M$. A downward water flow from a layer "i" can occur if water content θ_i

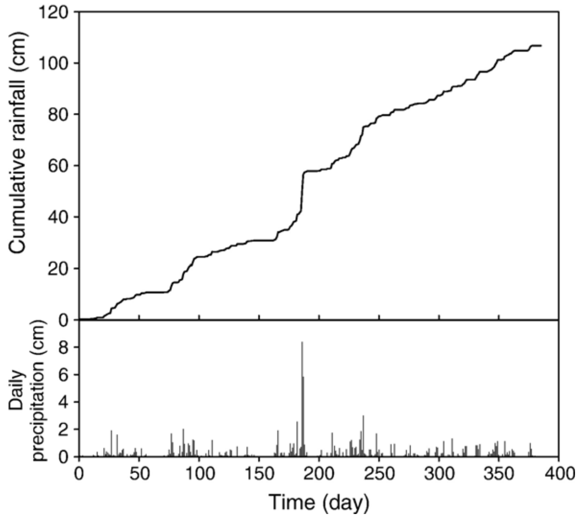

Fig. 5. Cumulative rainfall and daily precipitation during the experiment.

exceeds the value of water field capacity $\theta_{FC,i}$ of this layer. The value of flux q_i from the ith soil layer is calculated as:

$$q_i = \min(q_1, q_2)$$

$$q_1 = q_{i-1} + (\theta_i - \theta_{FC,i})\Delta z_i/\Delta t$$

$$q_2 = \min(K_{sat,i}, K_{sat,i+1}) \quad (15)$$

where q_{i-1} is the incoming water flux to ith layer, $K_{sat,i}$ is the saturated hydraulic conductivity of ith layer, Δt is the time interval set to one day.

The value of flux q_0 is calculated from the rainfall rate R as:

$$q_0 = \min(R, K_{sat,l}) \quad (16)$$

Fluxes q_i, $I=1, 2,\ldots, M$ are calculated recursively top-to-bottom. Fluxes may be corrected beginning from any internal layer to account for complete saturation of the layer.

The earlier version of this model was developed without accounting for evaporation (Guber et al., 1998). For the purposes of this work, the model was expanded to simulate the decrease of the layer water contents θ_i decrease due to evaporation and/or loss to the upward flow. The exponential equation describes the decrease in θ with time (Suleiman and Ritchie, 2003):

$$\theta_i = \theta_{r,i} + (\theta_{i,initial} - \theta_{r,i})\exp(-t/\tau) \quad (17)$$

where τ is the resistance parameter, $\theta_{r,i}$ is the residual water content. The daily change in water content is

$$\Delta\theta_i = -\frac{\theta_i - \theta_{r,i}}{\tau}$$

The value of τ increases with the depth z. Suleiman and Ritchie (2003) observed that a power function gave a good fit to relationships between τ and z for several soils and evaporation scenarios:

$$\tau = \tau_0 + az^b \quad (18)$$

where τ_0 is the value of resistance parameter at depth $z=0$, a and b are parameters of the evaporation model.

The simulated daily evaporation rate E is:

$$E = \sum_{i=1}^{n} \Delta\theta_i \Delta z_i \quad (19)$$

The number of soil layers n subject to evaporation is adjusted to make the value of E equal to the evaporation in the model input. An adjustment over those layers is made to provide the exact equality.

The set of the MWBUS model parameters includes the saturation water contents $\theta_{s,i}$, the field capacity values $\theta_{FC,i}$, the residual water content values $\theta_{r,i}$, and the saturated hydraulic conductivity values $K_{sat,i}$ for each layer, and the parameter of evaporation/upward loss submodel τ_0, a, and b.

4.2. Model parameters

A study of water retention along a 30-m trench in the same soil at the adjacent site (Mallants et al., 1996) was performed. Values of van Genuchten parameters were found from water retention measurements done at 5-cm long and 5.1-cm diameter cores with sand-box apparatus for capillary pressures of 1, 5, 10, 50, and 100 cm, and with pressure cell for capillary pressures of 200, 630, 2500, and 15,000 cm. Statistics of van Genuchten parameters are in the Table 2 (computed from digitized graphs). The variability of the van Genuchten parameters α and n was relatively high in all three horizons. There was a weak correlation between saturated water contents θ_s and $\log_{10}\alpha$. In all three horizons, and a moderate correlations between $\log_{10}\alpha$ and $\log_{10} n$. The same van Genuchten parameters determined in different horizons did not correlate. The field capacity value for the MWBUS model was taken as the water retention at 100 cm computed from the van Genuchten Eq. (13). This value did not have significant correlation with θ_s and θ_r (data not shown). The saturated hydraulic conductivity for simulations with both models was

Table 2
Statistics of van Genuchten parameters of water retention in samples along the 30-m trench

	$\theta_{r,Ap}$	$\theta_{r,C1}$	$\theta_{r,C2}$	$\theta_{s,Ap}$	$\theta_{s,C1}$	$\theta_{s,C2}$	lg $\alpha_{Ap}^{§}$	lg α_{C1}	lg α_{C2}	lg n_{Ap}	lg n_{C1}	lg n_{C2}
Min	0.000	0.000	0.000	0.348	0.330	0.379	−2.966	−2.947	−2.865	0.141	0.103	0.148
Average	0.040	0.015	0.044	0.411	0.363	0.431	−2.201	−1.951	−2.466	0.236	0.143	0.249
Max	0.083	0.075	0.101	0.484	0.424	0.502	−1.845	−1.536	−2.113	0.552	0.374	0.424
Coefficient of variation (%)	57.7	135.1	53.8	7.2	5.2	7.7	11.0	13.2	9.7	41.0	34.8	29.9
Correlation coefficients significant at 0.05 significance level												
$\theta_{r,Ap}$	1.000	–	–	–	0.268	–	−0.332	0.349	–	0.678	–	–
$\theta_{r,C1}$		1.000	–	–	–	−0.383	–	−0.338	–	–	0.851	0.254
$\theta_{r,C2}$			1.000	–	–	–	−0.381	–	−0.684	–	–	0.834
$\theta_{s,Ap}$				1.000	–	–	0.430	–	–	–	–	–
$\theta_{s,C1}$					1.000	–	–	0.558	–	–	–	–
$\theta_{s,C2}$						1.000	–	–	0.444	0.376	−0.285	−0.329
lg α_{Ap}							1.000	–	–	−0.453	–	−0.313
lg α_{C1}								1.000	–	0.282	−0.630	−0.333
lg α_{C2}									1.000	–	–	−0.899
lg n_{Ap}										1.000	–	–
lg n_{C1}											1.000	0.340
lg n_{C2}												1.000

§lg — the decimal logarithm.

estimated from texture and bulk density as suggested by Rawls et al. (1998). Values of K_{sat} were 40.3, 21.9, and 42.4 cm d^{-1} at depths from 0 to 25 cm, 25 to 65 cm, and 55 to 105 cm, respectively. Parameter l in the van Genuchten–Mualem equations was set to 0.5.

Fifty simulations of soil water flow were done with both models. Van Genuchten parameters of soil water retention were randomly sampled from the trench data for each layer to perform simulations with the HYDRUS-1D model. To run simulations with the MWBUS model, values of the saturation water contents and the residual water content values were randomly sampled from the trench data, values of the field capacity were computed from randomly chosen sets of van Genuchten data using Eq. (13) with $h=100$ cm. Measured daily precipitation and estimated evaporation of 0.86 mm were used to compute the boundary condition. The free drainage boundary at 150 cm was used with the HYDRUS-1D model.

5. Results and discussion

Simulated cumulative soil water fluxes are compared with measured values in Fig. 6 for three major wetting–drying cycles on days 112–143, 143–232, and 232–275. The average fluxes computed with the two models were not statistically different (t-test at $p<0.01$) at 15 and 55-cm depths for all three wetting–drying cycles. Only at the depth of 105 cm, average fluxes computed with the two models were significantly different for the days 112–143 and 232–275, and the HYDRUS model had a low accuracy for the days 112–143 whereas the MWBUS model had a lower accuracy for the days 232–275 at this depth (Fig. 6).

When the model errors were estimated at other time scales, the two models had similar accuracy. Fig. 7 shows the root-mean-square errors (RMSEs) of the average daily flux computed from 4, 8, 16, and 32 day-long time series of measured and simulated cumulative water fluxes. The time-scale dependencies of the RMSEs from the two were close (Fig. 7). Values of RMSE at the 55 cm depth were larger as compared with RMSE at other depths. This was probably related to the variability in measured flux values (see error bars in Fig. 6). Overall, the accuracy of HYDRUS-1D and MWBUS models was very similar with respect to the soil water flux values.

Unlike the accuracy, measures of information and complexity provided clear distinction between the two models. Fig. 8 shows information content and complexity parameters of rainfall and simulated soil water fluxes at the depth of 105 cm. Values of the metric entropy, and the mean information gain show that precipitation had very high randomness. For example, the metric entropy of precipitation is very close to one. For the two-symbol words this means that the distribution of observed states is close to the uniform distribution. Complexity of the precipitation time series is very low, and the precipitation time series are similar to the random process shown in Fig. 1. These results are analogous to the earlier results for precipitation in other humid regions shown in Fig. 2 (Lange, 1999a,b).

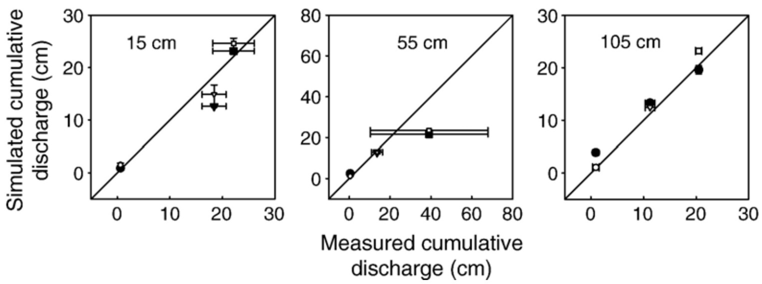

Fig. 6. Comparison of simulated and measured soil water fluxes over three major wetting–drying cycles on days 112–143 (●, ○), days 143–232, (θ, σ), and days, and 232–275 (■, □). Hollow and filled symbols show results from MWBUS and HYDRUS 1D, respectively.

The time series of simulated water fluxes have smaller information content as compared with precipitation and estimated soil water fluxes. This can be seen in Fig. 8 by comparing the metric entropy, and the mean information gain of simulated fluxes with those values for precipitation and estimated flux. The two flow models seem to serve as the information filters. Simulated redistribution within soil effectively smoothes the random precipitation input, and simulated fluxes are much less random than precipitation. We note that, unfortunately, the complexity and information measures could not be computed for the measured discharge because the discharge observations were done with varying frequency, and the discharge was accumulated during one to three days before being measured.

The HYDRUS-1D model had a tendency to generate soil water flux time series with less randomness as compared with the MWBUS model (Table 3). The average entropy and mean information gain over replicated simulations were significantly different ($p<0.001$ from the t-test). The MWBUS model had the range of information content measures much narrower than the HYDRUS-1D model. A possible explanation is that the soil water redistribution is simulated in much simpler fashion than in HYDRUS 1D and the signal-filtering, or de-noising, action of the former model with respect to the precipitation is weaker. The metric entropy ranges and the mean information content ranges overlapped for MWBUS and HYDRUS-1D and therefore the information content measures alone could not be used to discriminate between the two models.

The effective measure complexity and the fluctuation complexity show that complexity of simulated fluxes is higher than the complexity of the precipitation (Fig. 8). Simulated flux time series have a structure that may be related to the computational interdependence of soil layers. The larger number of computational layers and the larger number of the model parameters in HYDRUS-1D might contribute to the fact that this model generated more complex output water flux time series as compared with the MWBUS (Table 3). The MWBUS model had the range of the complexity measure values much narrower than the HYDRUS-1D model and generated less complex soil water flux time series. A possible explanation is that the larger number of water retention parameters in

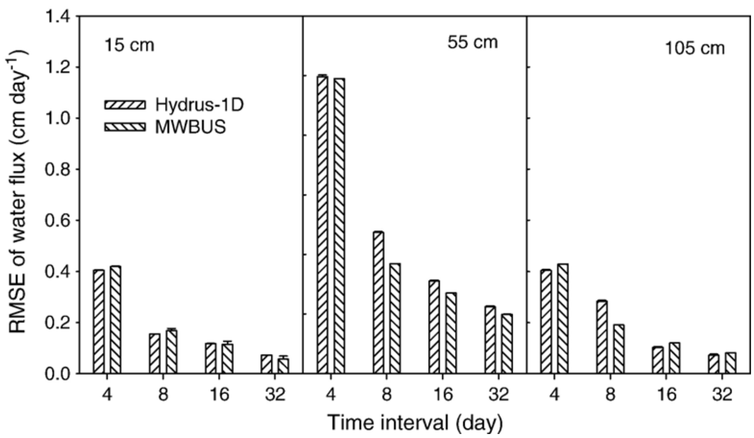

Fig. 7. Root-mean-square errors of simulated daily soil water fluxes computed as averages over time intervals shown at the horizontal axis.

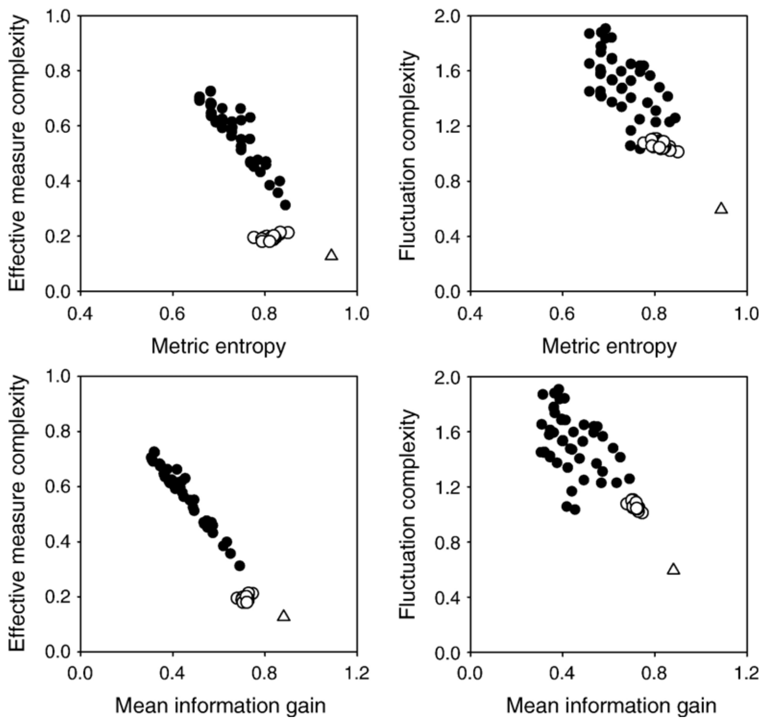

Fig. 8. Complexity and information content of rainfall and simulated soil water flux time series in layered soil profile at the 105-cm depth. Complexity is measured with the effective complexity measure and the fluctuation complexity, information content is measured with the metric entropy and the mean information gain; ● — simulations with HYDRUS-1D, ○ — simulations with MWBUS, ρ — rainfall.

HYDRUS-1D and their effect on the hydraulic conductivity introduces a structure in water fluxes at soil profile bottom. The metric entropy ranges and the mean information content ranges overlapped for MWBUS and HYDRUS-1D and therefore the complexity measures alone could not be used to discriminate between the two models.

The good model discrimination was achieved when both information content and complexity measures are used to characterize the simulated time series. Using the effective measure complexity in combination with the mean information gain was the most efficient way to discriminate models in this work (Fig. 8). The continuum mechanics representation of soil water flow in HYDRUS-1D resulted in more complex output with less randomness.

The separation of the model outputs in the coordinates 'information-complexity' depended on the depth where the soil water fluxes were computed. Mean information gain, fluctuation complexity, and effective complexity measure are compared in Fig. 9 at depths of 15, 55, and 105 cm for HYDRUS and MWBUS models. Ranges of the mean information gain and the measures of complexity depended on the depth. Complexity of the flux simulated with the HYDRUS-1D model at 15 cm was less at 15 cm than at 55 cm and at 105 cm. The range of the mean information gain increased as the depth increased when the HYDRUS-1D was used. With MWBUS model, a decrease in the range of both complexity measures and the information content measure was observed as the depth increased. No increase in average complexity was

Table 3
Average values of the information theory measures computed for soil water flux time series simulated with HYDRUS-1D and MWBUS models

Information theory measure	Layered soil		Homogeneous soil profile	
	HYDRUS-1D	MWBUS	HYDRUS-1D	MWBUS
Metric entropy	0.73±0.05[¶]	0.81±0.01	0.70±0.05	0.82±0.02
Mean information gain	0.44±0.10	0.71±0.01	0.39±0.10	0.72±0.02
Effective complexity measure	0.58±0.10	0.19±0.01	0.61±0.10	0.20±0.01
Fluctuation complexity	1.52±0.21	1.07±0.03	1.70±0.15	1.06±0.04

[¶]The "±" sign separates average and standard deviation.

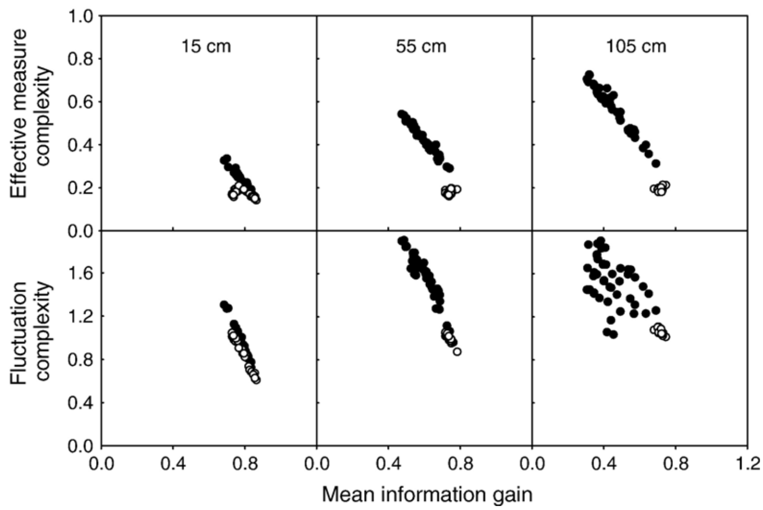

Fig. 9. Complexity and information content of simulated soil water flux time series in homogeneous soil profile at the 15, 55 and 105 cm depth. Complexity is measured with the effective complexity measure and the fluctuation complexity, information content is measured with the mean information gain; ● — simulations with HYDRUS-1D, ○ — simulations with MWBUS.

seen as the depth increased when the MWBUS was used. A trend of the decrease in average information content depth can be observed with in Fig. 9 for both models. The mean information gain at the 15-cm depth is close to the one of the precipitation. As the depth increases, the mean information gain decreases. The ability of the flow models to serve as information filters increases with depth. Fig. 9 shows that it is not possible to distinguish the two models with data on information content and complexity at the 15-cm depth (Fig. 9). The differences between models become substantial at larger depths, probably because more information filtering occurs as the depth increases.

An insight in the differences in complexity and information content can be gained by considering the probabilities of symbolic words and transitions in symbolic strings representing rainfall and simulated water fluxes. Table 4 shows those probabilities computed for precipitation and for the typical model outputs. All these time series show the persistence in water fluxes. The probability of today and tomorrow fluxes to be both less than median, or to be both greater than median is larger than probabilities of switches from less than median to the larger than median or vice versa. However, the probability of switch from the ‘less than median’ to the ‘greater than median’ state in simulated fluxes is smaller than precipitation. The continuous sequences of ‘larger than median’ or ‘smaller than median’ days are shorter in precipitation than in simulated soil water fluxes. This may be related to the fact that large volumes of rainfall accumulate in soil and it takes some time to discharge the water through the bottom of soil profile. Because the redistribution of soil water in the MWBUS model is instantaneous, the periods of low (or zero) bottom flux

Table 4
State and transition probabilities for the symbol strings representing time series of precipitation and simulated soil water fluxes

	Precipitation				MWBUS model				HYDRUS-1D model			
State “j”[¶]	‘00’	‘01’	‘10’	‘11’	‘00’	‘01’	‘10’	‘11’	‘00’	‘01’	‘10’	‘11’
	State probabilities p_j											
	0.347	0.151	0.154	0.347	0.576	0.107	0.107	0.209	0.407	0.039	0.042	0.512
State “i”	Transition probabilities $p_{i\to j}$											
‘00’	0.246	0	0.102	0	0.493	0	0.081	0	0.372	0	0.037	0
‘01’	0.099	0	0.052	0	0.081	0	0.026	0	0.034	0	0.005	0
‘10’	0	0.039	0	0.113	0	0.034	0	0.073	0	0	0	0.042
‘11’	0	0.113	0	0.236	0	0.073	0	0.136	0	0.039	0	0.471

[¶]State ‘00’ — less than median value today and tomorrow, state ‘01’ — less than median value today, greater than median value tomorrow, state ‘10’ — greater than median value today, less than median value tomorrow, state ‘11’ — greater than median value today and tomorrow.

are highly probable compared with other time series. The HYDRUS-1D model has the longest periods of consistently larger than median or consistently lower than median fluxes. This model generates relatively smooth fluxes because the randomness is filtered during the water redistributions. Therefore, the corresponding time series have the smallest information content. On contrary, the precipitation time series is closer to the uniform distribution than the model outputs, and thus has the largest information content expressed as the metric entropy. Similarly, the presence of relatively large transition probabilities causes appreciable information gains in precipitation time series. Low transition probabilities make transitions non-informative in model outputs and the mean information gain is much lower in simulated flux time series as compared with precipitation. The complexity depends on the variability among transition probabilities. High asymmetry of the transition probabilities distribution in the HYDRUS-1D output makes them the most complex.

An increase in complexity of the conceptual soil water flow models is often being associated with considering a layered flow domain instead of a single homogeneous layer. For one, this definitely causes an increase in the number of parameters, as each layer has its own set of soil hydraulic properties. We ran fifty Monte Carlo simulations of soil water fluxes for the single soil homogeneous layer. Hydraulic properties of this layer were the same as they were for the topsoil layer in above simulations for the layered soil. Information content and complexity for the single layer simulations are shown in Fig. 10, and statistics of the information theory measures are shown in Table 3. Results are very similar to the results for the layered soil profile in Fig. 8. The distributions of complexity measures were slightly tighter for the single layer. When the graphs in Figs. 8 and 10 were superimposed (not shown), they were mostly indistinguishable. The information content and complexity of simulated soil water fluxes appeared to be affected by the type of water flow transport mechanism descriptions rather than by the variation of parameters within the flow domain.

There seem to exist several interesting avenues of research in assessment of information content and complexity of model output time series. First, the information theory offers a variety of other measures to assess information content and complexity of systems with a finite number of states For example, Fraser (1989)

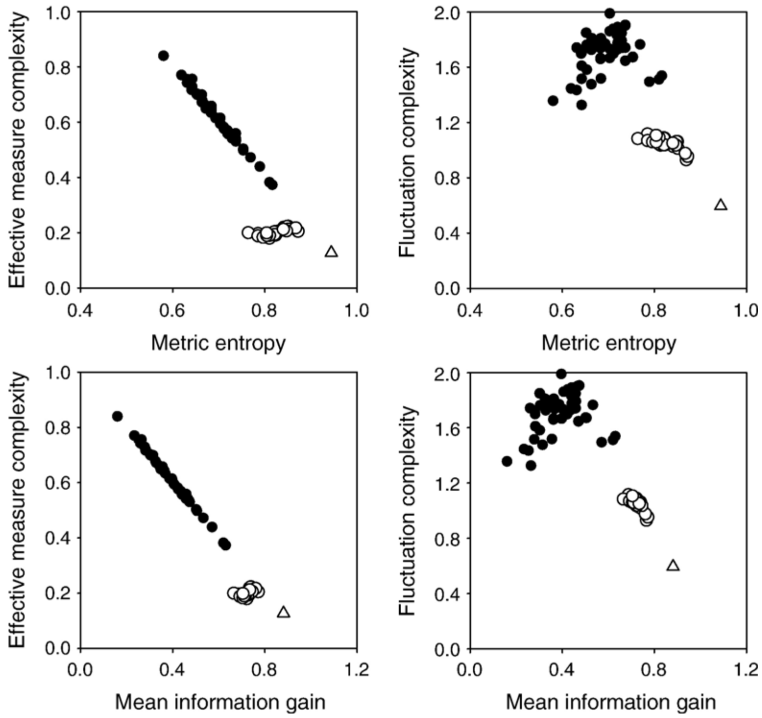

Fig. 10. Complexity and information content of rainfall and simulated soil water flux time series in homogeneous soil profile at the 105-cm depth. Complexity is measured with the effective complexity measure and the fluctuation complexity, information content is measured with the metric entropy and the mean information gain; ● — simulations with HYDRUS-1D, ○ — simulations with MWBUS, ρ — rainfall.

proposed to use the mean mutual information to measure how much information is in the dependency, or correlation, of two successive words. Rényi (1961) introduced a generalization of the Shannon entropy — the Rényi entropy of the order α that allows weighing rare or frequent words differently. High probabilities are strengthened compared to low probabilities for $|\alpha|>1$. If $|\alpha|<1$, then the lower probabilities are strengthened. Wolf (1999) proposed to use differences of Rényi entropies of conjugated orders as a measure of complexity. Pincus (1995) suggested using the approximate entropy when classical statistics did not show clear distinction. It is possible that the choice of measures of information content and complexity to discriminate models may depend on the type of model and the type of model output.

Another issue of interest to explore is the relation between the information content and complexity of soil water model outputs and the ability of soil water models to serve as hydrologic drivers (or vehicles) in simulating solute transport or energy balance. Output of two-dimensional flow models can also be analyzed with information theory measures (Andrienko et al., 2000).

Temporal scale presents yet one more facet of the information content and complexity evaluation. The full reverse-parabola-like complexity–information curve (as shown in Fig. 1) has not been reproduced in this work. The calculated "mean information gain-fluctuation complexity" points are mostly on the descending branch of that curve (Figs. 8 and 9). Some part of the dynamics could be lost in randomness of a relatively coarse temporal sampling, and finer scales may yield better reflection of the system dynamics and even better model discrimination (Wolf, 1999).

Two conceptually different soil water flow models gave the same accuracy in predicting soil water fluxes in this work. Such non-uniqueness of model structure becomes a norm rather than an exception. A comprehensive contemplation on the non-uniqueness of modeling in environmental sciences was recently presented by Beven (2002, 2003). In the past, the attitude was that if a model is comprehensive enough, it would be possible to represent the site uniqueness with a specific set of model parameters. Recently, there has been a major increase in detailed studies that, generally, have revealed a complexity in flow pathways due to heterogeneity at different scales and interactions between geometry of the flow domain and prevailing hydraulic gradients including both "preferential flow" and "stagnant zones." Complexity of flow pathways may be easily perceived but difficult to represent in mathematical terms without making strong simplifying assumptions. This implies that many different model structures could be consistent with available observations. Beven (2000) argues that no matter how intensively a site is studied, there is a wide range of models and parameter sets for each model that will yield acceptable simulations. Such multiplicity of models is simply a summed expression of the limitations to current models in representation of flow systems, limitations of measurement techniques with respect to scales of public interest, and limitations in defining initial and boundary conditions. One cannot also exclude the possibility that there still exists a lack of fundamental understanding in fluid and chemical transport processes in the environment, and this precludes building of widely applicable models.

If there is a wide range of models and parameter sets for each model that will yield acceptable simulations, then what can be an approach to model selection? Existing approaches to the model selection are based on the availability of input data, on previous experience, or on physically meaningful model performance with reasonable scenarios using, i.e., the Generalized Likelihood Uncertainty Estimation (GLUE) methodology (Beven, 2002). However, an impeccable way to select "the model" is unknown. Using the information theory to discriminate models may give additional insights in their performance and make a site-specific model pick.

Overall, more complex simulated soil flux time series were obtained with the HYDRUS-1D model that was perceived to be conceptually more complex than the WMBUS model. An increase in the complexity of water flux time series occurred in parallel with the decrease in the information content. Using both complexity and information content measures allowed us to discriminate between the soil water models that gave the same accuracy of soil water flux estimates.

Acknowledgements

This work was partially supported through the Interagency Agreement RES-02-008 "Model Abstraction Techniques for Soil Water Flow and Transport. We are grateful to Dr. F. Wolf and two anonymous reviewers for their valuable comments on the early version of the manuscript.

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