Book of Abstracts
International Workshop on Catchment scale Hydrologic Modeling and Data Assimilation

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Preface

This volume brings together the abstracts of a special three-day workshop on Catchment-scale Hydrological Modeling and Data Assimilation held at De Wageningse Berg conference center in Wageningen, the Netherlands, between September 3rd and September 5th, 2001. The workshop was organized in the framework of a EU funded research project on Data Assimilation Within a Unifying Modeling Framework for Improved River Basin Water Resources Management (EVK1-CT-1999-00022).

The objectives of the workshop were to bring together experts in catchment-scale hydrological modeling to discuss new modeling strategies and the potential of using advanced data assimilation methods to improve parameterization and predictability of distributed and semi-distributed catchment-scale hydrological models.

Scientific progress and strategic planning in watershed management rest on being able to make the best use possible of advanced simulation models and the large amounts of environmental data that are increasingly being made available, owing to innovations in instrumentation for field or in-situ monitoring and in airborne and satellite remote sensing techniques. There is therefore an urgent need for a formal methodology to integrate these data with models in an optimal way so as to improve the accuracy of predictions and the reliability of scenario analyses based on the data and simulations.

The fundamental operative unit for the implementation of water resources management strategies is the catchment or the river basin. Models developed at such large scales are either too simple or too complex to take advantage of advanced data assimilation procedures, and thus there has not been much progress in applying these methods in hydrology, as compared to their successful development and operational use in ocean and meteorological sciences. What is needed are "smarter" distributed models that include enough physical realism but at the same time are computationally efficient and can handle the large amounts of additional spatial information at the catchment scale.

The workshop is organized around six sessions:

1. New approaches to catchment-scale modeling
2. Data assimilation methods
3. Spatial data and distributed models

4. Model calibration
5. Remote sensing and hydrological models
6. Data assimilation in hydrological modeling

The abstracts presented here are listed in the order as presented during the workshop. A special issue of Advances in Water Resources which will include several contributions at the workshop is under preparation.

We are grateful for the financial and organizational support provided by the following Dutch and international organizations: the Hydrology and Quantitative Water Management group and the Department of Environmental Sciences of the University of Wageningen, the Koninklijke Nederlandse Academie voor Wetenschappen (KNAW, Royal Dutch Academy of Sciences), the 5th Framework Programme of the European Commission (Directorate I - Preserving the ecosystem: environmental research), and The International Hydrological Programme of UNESCO. The smooth running of the workshop owed a lot to the hard work of a number of volunteers - our sincere thanks to them, and especially to Ewa Wietsma, Annemarie Hofs and Henny van Werven.

We thank all those who made presentations at the workshop. We take the opportunity to thank our panel of the scientific committee for reviewing the content of the abstracts.

August, 2001

E. Emiel van Loon
Peter A. Troch

1 New approaches to catchment scale modeling
Chairman: C. A. Paniconi

New approaches to predictions of ungauged catchment responses

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The fundamental operative unit for the implementation of water resources management strategies is the catchment or watershed. At the present moment hydrologists do not have the ability to make predictions of large catchment responses, using models that (1) are physically-based at the scale of the catchment, and (2) with parameters that can be estimated a priori without the requirement of calibration, ie., ungauged catchments. Past debate in this area has been over the relative advantages and disadvantages of distributed, physically-based models versus lumped conceptual models. This debate has not produced the advances in our modeling capability for ungauged catchments.

This talk will focus on new, potentially powerful approaches that can be utilised to build hydrological models directly at the scale of catchments, having the advantage that they are both physically-based, and parsimonious in terms of data and computing requirements. The upward approach attempts to combine, by mathematical synthesis, the empirical facts and theoretical knowledge available at a lower level of scale into theories and models capable of predicting the responses at the higher level.On the other hand, the downward approach strives to find a concept directly at the level or scale of interest and then looks for the steps that could have led to it from a lower level or scale.

An example of the upward approach is the work of Reggiani et al. [134, 133], in which the whole watershed is divided into smaller entities called representative elementary watersheds (REWs).An averaging procedure is employed to derive balance equations for mass, momentum, energy, and entropy at the scale of the REWs. This is supplemented by a constitutive theory, based on 2nd law of thermodynamics, to guide the parameterization of unknown exchange fluxes that appear in the balance equations. This results in a semi-distributed ensemble of interconnected discrete points replacing the fully distributed description of the watershed. Each point represents a channel link and its contributing surface and subsurface flow regions. The resulting equations are subsequently assembled for all channel links of the watershed and solved simultaneously for water depths, velocities, and saturations in each zone. Examples of the application of this approach for the construction of models can be found in [135, 136].

The downward approach involves learning from observed spatial and/or temporal patterns of hydrologic response in a systematic manner. Examples of the downward approach are the recent work in [56, 86, 7, 47]. A basic assumption in the approach is of an evident hierarchy of controlling influences relating climate-landscape interactions to the prediction of hydrologic responses at various space-time scales of interest. Relatively simple approaches are often adequate to capture the essence of water balance at large time and space scales, provided they take into account the primary controlling variables of precipitation, potential evaporation and soil storage capacity. When greater levels of prediction are required

(i.e. at smaller spatial and/or temporal scales), then consideration must be given to the inclusion of additional variables and processes, in order to address the more subtle causes of variability. Testing of hypotheses and theories with respect to climate and landscape controls must be carried out in respect of key signatures of variability at the monthly, daily and hourly time scales, and at correspondingly small space scales (catchments, hillslope, plot etc.).

The talk will give an overview of the recent advances in each approach, and the prospects for combining both approaches to assist in the development of models for predictive purposes. Data is fundamental to both approaches.For the upward approach, considerable work remains to be done to develop catchment-scale parameterizations of the various exchange fluxes, including especially the effects of sub-grid variability, based on readily available datasets such as DEMs, soil maps, remote sensing information and new field surveys and experiments.The downward approach, is by definition, a highly data-dependent approach, and currently available datasets of all water fluxes as well as catchment parameters, must be used in a systematic, hierarchical manner to learn as much as possible from available data about the functioning of the catchment.

Thus both approaches can benefit from sophisticated data assimilation methods, that account for (1) the natural organisation of catchments in space, in terms of stream network, hillslopes, soil catena, climatic variations etc., and (2) organisation of rainfall-runoff data in the temporal domain in terms of natural signatures of variability, such as inter-annual variability, seasonal or intra-annual variations, the flow duration curve and the flood frequency curve. The talk will cover the requirements of efficient data assimilation schemes that can maximise the use of these natural signatures in both time and space. In this sense, the requirements of data assimilation schemes in catchment hydrology are much more demanding, compared to what is presently used in atmospheric or oceanic models.

Application of POWER, a representative elementary watershed model, to a generic watershed

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Recently, a new approach for watershed modeling has been developed by Reggiani et al. [134, 133]. In this approach the watershed-scale balance equations for mass, momentum, energy and entropy are obtained by averaging the corresponding point-scale equations over regions called Representative Elementary Watersheds (REW).

The REWs are well-defined non-uniform spatial entities that are organized around the topological structure of the stream channel network, such that the ensemble of REWs constitutes the whole watershed. Each REW may be seen as a sub-watershed; its boundary coincides with topographic divides delineating a well-defined area of the land surface that captures precipitation and delivers it to the river channel. Within the volume making up a REW, five different flow zones are distinguished: (1) unsaturated flow, (2) saturated flow, (3) saturated overland flow, (4) concentrated overland flow, and (5) channel flow. For the unknown exchange fluxes across boundaries between the zones and between the REWs, constitutive relationships have been developed in a physically consistent manner.

Variables and properties associated with an REW are spatially lumped quantities that vary only in time. The governing equations of the model constitute a system of coupled ordinary differential equations, yielding a drastic simplification of the description of the system compared with conventional physically based runoff models, such as Mike-SHE.

Following the above approach we have developed a model called POWER. The resulting model has the advantage that it is based on physical principles and in addition requires much less input data and computer resources than traditional grid-based watershed models. Because of the reduced complexity and lower computational costs, it has favourable properties for combination with data assimilation techniques.

In recent work [135, 136], Reggiani et al. applied the REW approach to two simplified cases: subsurface flow in a single REW, and flow in a stream channel network.

In this presentation we apply the model to a real-world catchment. We study the response of the watershed to a number of rainfall events and compare the results with available data. Furthermore, we consider a number of generic aspects of the REW modeling approach. For example, we investigate the effects of the applied spatial discretization in terms of the number of REWs on the computed results, and we perform a sensitivity analysis for a number of model parameters.

A new approach for using radar rainfall data in catchment hydrology

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In the last decade there has been an increasing interest among hydrologists in the utilization of meteorological radar data for runoff prediction. The high spatial and temporal resolution of the radar rainfall data have the potential to solve the inaccurate representation of the rainstorm over the catchment by the rain gauges data, which is one of the a weakest points in rainfall-runoff modeling. Numerous studies examined how to use radar data in hydrology, but no clear breakthrough is evident. Although many studies demonstrated improvement in runoff prediction by using radar rainfall data, others, claimed that the large error associated with the radar data could generate high inaccuracies in forecasted flows. The basic reason for the large errors is that the meteorological radar does not measure directly rainfall intensities but indirectly estimates their value from backscattered radiation by using remote sensing techniques. The benefit of the high-resolution radar rainfall data is therefore questioned occasionally. The purpose of this research is to introduce a new approach for the use of radar rainfall data for estimating catchment runoff that alleviates this difficulty.

The general view Two key issues form the basis of this research: 1. Currently, the common strategy for using the radar in hydrological applications is to apply the data to existing hydrological models, which are adjusted to receive the high-resolution radar rainfall data instead of the conventional rain gauge data. Consequently, the radar data are used according to concepts, assumptions, and methodologies that were developed and applied to sparsely measured rainfall data. However, it should be recognized that rain gauge and the radar data are essentially different. Specifically, radar data on rainstorm evolution, structure, location and movement, was never available before, and should be viewed as a new and different type of rainfall data rather than merely representing a dense network of rain gauges. Therefore, new approaches and methodologies should be developed for using these data in hydrology. 2. Rainfall data can be used with models at different time and space scales. Radar data are often used in hydrological models at the most detailed resolution available; obviously, at this scale the data contain the maximum amount of information. However, considering the large error in radar rainfall at the small scale, and taking into account the integrative nature of the hydrological processes, this is not necessarily the best strategy. The optimal scale is the one at which the radar data contain a sufficient amount of information for estimating the catchment outlet runoff with adequate accuracy. The identification of this scale is an essential stage, prior to modeling.

The research goals The current research concentrates on the time-scale of small catchments (10-100 km^2) in semi-arid and arid climates. The research objectives are: 1. To develop a method for identifying the characteristic time scale of hydrological catchment response (the response time scale - RTS). This scale-identification must be a pre-modeling stage, and therefore, the method for determining the RTS is based on analysis of radar rainfall and runoff observations and does not assume a specific rainfall-runoff model. 2. To determine the dependence of the RTS on catchment characteristics. These relations are important from the theoretical point of view, to gain a better understanding of the catchment hydrological response, and from the practical point of view, for future use of this approach in areas where runoff measurements are not available. 3. To develop a rainfall-runoff model at the response time scale for a selected catchment. The input is radar rainfall averaged over the entire catchment area at its pre-determined response time scale and the output is the outlet runoff.

The Response Time Scale (RTS) The hydrological response of the catchment is the transformation of rainfall over the catchment into runoff at its outlet. Given a general system that receives an input time series and generates an output time series, one can characterize the time scale of the system by measuring the amount of smoothing that is performed on the input in this transformation. This characterization involves analysis of the two time series, without assuming a specific model for representing the system. The RTS measures the amount of smoothing needed to make the rainfall input hyetograph become similar to the runoff output hydrograph. The RTS algorithm is based on comparing catchment averaged radar rainfall graphs represented at different time scales with the corresponding runoff hydrograph, and selecting the time scale at which the smoothness of the two graphs is the same. The algorithm can be applied to a single rainfall-runoff event or to a group of events. The RTS algorithm is applied to four small (10-100 km^2) catchments in Israel. The catchments have different land-use (urban, rural and natural) and climate (semi-arid and arid). A stable RTS value is found for each of the four catchments, indicating that the response time scale is an intrinsic property of the catchment. The urban and arid catchments are characterized by short time scales (5-30 min), while the two rural catchments are found to have a slower hydrological response (1-3 hours).

The relationships of the RTS to catchment characteristics The hydrological response of the catchment is described by a non-calibrated, physically based hydrological model that is applied to one of the four catchments. The radar rainfall data are used to obtain the computed runoff hydrographs, and these computed data are then used to derive the RTS of the modeled catchment. The effect of several catchment parameters (such as length, slope and roughness of hillslopes and channels) on the RTS is examined by altering each parameter and deriving the RTS for each case. The effect of the different parameters on the time scale characteristics of the catchment hydrological response is investigated. Special emphasis is placed on comparison of hillslope vs. channel processes. The results indicate that the effect of hillslope processes on the response time scale is greater than the effect of the channel processes.

Estimating catchment runoff using radar data smoothed at the RTS Based on

comparison of radar rainfall graphs smoothed at the RTS with measured outlet runoff graphs, an empirical rainfall-runoff model is developed for the selected catchment. The model is calibrated with data from one group of events and is then tested with data from a verification group of events. A reasonable fit is found between computed and measured runoff, considering the large error that exists in the runoff data.

Summary A method for identifying the RTS of small catchments, based on radar and runoff measurements is presented. Stable values of the RTS were found for the four studied catchments. The RTS of the urban and arid catchments are small relative to the RTS of the rural catchments. The relationships of the RTS to catchment characteristics are studied using a hydrological model. The results indicate that the effect of hillslope processes in large as compared with channel processes. A rainfall-runoff model is developed for one selected catchment for estimating outlet runoff based on radar rainfall data smoothed at the RTS. The model performance is found to be adequate.

Hydrologic Modeling of Extreme Floods

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Extreme floods represent an important modeling challenge for which it is crucial to utilize the simplest model representations that capture the dominant controls of extreme flood response. For extreme floods, the spatio-temporal structure of rainfall and drainage network structure often play a fundamental role. The integrated hydrologic and hydrometeorological processes that control extreme flooding are examined through modeling studies of 8 extreme flood events in the United States. The elements of the hydrologic model are a Hortonian infiltration model (the Green-Ampt model with moisture redistribution) and a semi-distributed GIUH-based network response model. Rainfall fields are estimated at 1 km horizontal scale and 5 minute time scale from volume scan reflectivity observations from WSR-88D radars (along with rain gage observations). For each event, discharge time series at 15 minute time scale are available from one or more stream gauging stations. The basin scales of interest range from approximately 10 to 1,000 sq.km. Each event is characterized by extreme rainfall (150 - 700 mm) during a 2 - 6 hour time period. Event runoff ratios are larger than 0.5 and in several cases close to 1. Basin settings range from the high-gradient sub-tropical forests of central Puerto Rico to the low-gradient semi-arid plains of Nebraska. Return intervals of peak discharge values for the 8 events range from approximately 50 years to longer than 1000 years.

Applying Artificial Neural Networks to model surface flow contributions from the ungauged parts of the Kafue subcatchment (Zambia)

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Introduction Zambia relies quite heavily on surface water for hydroelectric power generation, irrigation and water supply. The recurrence of partial droughts and/or droughts is making it difficult to manage the water to meet the various competing water demands adequately and efficiently. Thus, the need for modeling of rainfallrunoff and streamflows of both the gauged and the ungauged sections of a catchment to be able to quantify the available water resource is an essential first step. A conceptual rainfallrunoff (CRR) model would be ideal since conceptual watershed models are generally reliable in forecasting the most important features of the hydrograph, such as the time and height of the peak, and volume of flow [147]. However, the implementation and calibration of such a model can be difficult; requiring sophisticated mathematical tools [45], significant amounts of calibration data [183], and some degree of experience with the model. This paper presents a methodology which can be called "semi conceptualsystem theoretic". It consists in the first place in deriving the tributary flow (ungauged) and direct runoff (from rainfall falling very close to and directly onto the main channel and reservoir). This derivation is done in a conceptual manner using reservoir routing approach [29]. The derived combined tributary and direct runoff (TrRO) is then taken as the desired/target output to be mapped in system theoretic modeling, by using artificial neural networks (ANNs).

The study sub-catchment and data The study subcatchment stretches from the Kafue Hook Bridge (KHB) to the confluence of the Kafue and the Zambezi rivers, which is the middletolower (Kafue Flats) basin and is approximately 50,000 km^2. It wholly lies within an area known as region 2, with annual mean rainfall of 8001000 mm. About 70% of the electric power is generated in the lower part of the catchment at the Kafue Gorge hydroelectric plant (KafGHEP). Here are found two sizeable manmade reservoirs, the ItezhiTezhi (Itezhi) and the Kafue Gorge (KafG) with 5000 Mm^3 and 700 Mm^3 live storage respectively and one natural lake Natural Reservoir (NR). The available data are hydro-meteorological variables from a number of stations distributed near and within the sub-catchment. The length of historical records of daily readings of each station vary, but on average they span about 15 years up to as recent as 1995/96 hydrological year. Some of the measured variables are rainfall, river discharge, evaporation, temperature, reservoir levels, reservoir releases, and turbine intake (for electric power generation).

Methodology First the sub-catchment is subdivided into three subsystems whereby each one is characterised by one reservoir. If there is a meteorological station that is somewhat centrally located, its records can be taken to be representative of the subsystem otherwise a weighted average using the Thiessen Polygon is used. Here the first subsystem

(Itezhi subsystem) which is about 10,500 km^2 is presented in detail. At the upper end of this subsystem is a gauging station at KHB, there are few tributary streams that are known to be ephemeral, and the Itezhi reservoir with its outlet structures. The relevant hydro-meteorological variables on which values are available such as inflow (Inf KHB), evaporation (Evap), levels of abstraction (Abst), daily changes in storage (DS), outflow from the reservoir (Out Itz), an estimation of percolation losses (Perc) were entered into an Excel spreadsheet to derive the unknown combined tributary and direct runoff (TrRO). To do this a simplified reservoir routing equation in which dynamic effects are neglected, thereby reducing it to a continuity equation, is used. According to this equation, the difference between the inflow and outflow is equal to the rate of change of volume of water stored (S), in the reservoir. A finitedifference approximation may be written as

$$\frac{\Delta S}{\Delta t} = \overline{I} - \overline{O} \tag{1.1}$$

in which $\overline{I}$ and $\overline{O}$ indicate mean values using the time interval (Δt=1day) and where

$$\begin{aligned} \overline{O} &= Abst + Evap + Out_{Itz} + Perc \\ \overline{I} &= Inf_{KHB} + TrRO \end{aligned} \tag{1.2}$$

By combining 1.1 and 1.2 and rearranging the terms we get

$$TrRO(t) = \overline{O}(t) + \frac{\Delta S}{\Delta t} - Inf_{KHB}(t) + \xi \tag{1.3}$$

were ξ is the combined effect of model and data errors [81] and (t) shows that both inputs and output are time series. The probable inputs to the system theoretic, in our case ANN models, are rainfall $R(t)$, $R(t-1)$; previous time-step outputs $TrRO(t-1)$, $TrRO(t-2)$ and evaporation $E(t)$. Correlations of these inputs and output are calculated in form of a correlation-matrix so the relative contribution of each input to the output could be seen at glance. The stage was now set to apply the ANNs which are a flexible mathematical structure capable of identifying complex nonlinear relationships between input and output datasets. The rainfallrunoff (RR) process is highly nonlinear, time varying, spatially distributed and not easily described by simple models [128, 71]. The system theoretic approach is generally based on difference or differential equation models to identify a direct mapping between the inputs and outputs without detailed consideration of the internal structure of the physical process [78, 63].

The inputs and output time series were partitioned in three pattern sets: training, validation and testing in such a way that some earlier, middle and recent data points were included in each set, to remove this bias due to longterm changes. By partitioning the data series some impartiality in evaluating the prediction performance is builtin, in that data for different periods are used for "training" (modeling), "testing" (prediction), and validation. All these sets are of the form $\{x_1(t), x_1(t), \ldots, x_1(t); d_t : t_0 \leq t \leq M\}$ in which $x_i(t)$, are the inputs while $d(t)$ is the desired output $TrRO(t)$. Some earlier work in neural

network research has shown that a three layer (Input layer:1Hidden layer:Output layer) feed-forward ANN through back-propagation of errors is capable of mapping and generalising any mathematical function. The above inputs (in normalised form, i.e. ranging from 0 to 1) in various combinations were presented to a host of one hidden layer feed forward – back-propagation ANNs for training using MATLAB routines. For each combination of input patterns the number of neurons in the hidden layer was varied from 2 to 20 while the pertinent global 'goodnessoffit' statistics for each satisfactorily trained network were noted. The training method used is LevenbergMarquardt 'TRAINLM', in which an early stopping criteria is incorporated to safeguard against overfitting. In each step in the training phase, the network is required to predict the next value in the time sequence. The error between the value predicted (by the network) and the value actually observed (in this case derived) is measured and propagated backwards along the feed-forward connections. During training the evolution of the mean squared error MSE(training) is plotted against "epochs" (cycles of presentations of all training inputs). Some of the 'goodnessoffit' statistics that were used to select a bestfit network for further tests are the ratio of the standard error of estimate (S e) to the standard deviation of TrRO (S), (S_e/S) also called the noisetosignal ratio [160]; the percent volume error (in addition to these, parsimony (to have as few parameters as is necessary) as a guiding principle was taken into account. [131] talking of ANNs note, "These new technologies, however, require evaluation against conventional models and statistical tools, in order to determine their relative performance...". To evaluate the shortlisted ANNs further for their forecasting capabilities they are compared with ARMAX (autoregressive moving average with exogenous input) models. ARMAX models have been widely used for watershed modeling because of the ease with which they can be developed [185]; and they have been found to provide satisfactory predictions in many applications [20]. The model outputs of both ANNs and ARMAX are regressed with the observed/derived $TrRO(t)$ for a few selected prediction horizons and the regression coefficient (R) and mean squared error (MSE) as performance statistics are noted. In almost all cases the ANN models generated better statistics. It was also clear from both visual and statistical points of view that ANNs did not deteriorate as rapidly as the ARMAX models as the prediction horizon increased hence confirming the robustness of ANNs for long term forecasting. It, therefore, can be seen that ANNs are a viable alternative and/or complimentary approach to conventional catchment modeling techniques.

Evaluation of hydrological modeling at the catchment scale using NAM

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In recent years, water resources studies have become increasingly concerned with aspects of water resources for which data are not directly available or very limited. With this respect, hydrological simulation models are often used for the physically based description of surface waters. They can form a solid basis for decision management regarding water resources. In this study, the applicability for integrated watershed management of the lumped conceptual rainfall modeling system NAM (Danish Hydraulic Institute) was tested. Meteorological data and stream flow measurements were used for six sub-catchments in the Belgian River Dender basin (1384 km^2). Calibration and validation of the models were performed on the basis of new concepts. To model the ungauged catchments, a correlation has been searched between the different sub-catchment characteristics (land use, soil characteristics and drainage conditions) which were analysed by GIS and model parameters. To evaluate the model results, the sensitivity of the results to rainfall data from measurement stations at different distances from the catchment and with different measuring accuracy was studied. Also the importance of the daily volume corrections on the hourly rainfall time series was analysed. The influence on the accuracy of the model results is studied based on a comparison of independent hydrograph maxima and minima, and on a comparison of the frequency distribution derived from a long term simulation.
Keywords: rainfallrunoff, modeling, calibration, GIS, regionalisation, sensitivity analysis, extreme value analysis

NAM is an abbreviation meaning precipitationrunoffmodel. The Hydrological Section of the Institute of Hydrodynamics and Hydrological Engineering has developed this modeling system at the Technical University of Denmark. In this study NAM is implemented and evaluated for the different sub-catchments of the river Dender watershed in Belgium. The river Dender is located in the Flemish region of Belgium to the west of Brussels. The Flemish part of the Dender catchment area is divided into 12 hydrographic sub-catchments (zones). On the basis of the six available discharge measuring stations, NAM is calibrated for six sub-catchments in the Dender basin. Meteorological and streamflow data are used for the period between January 1, 1989 and December 31, 1993. Model input consists of hourly rainfall data at the meteorological station of Ukkel, which is located at 30 km from the catchment centre. The storm volumes are corrected on the basis of daily rainfall data at three meteorological stations inside the catchment by using the Thiessen polygon method. Because of the time resolution of 1 day, the same correction factor has to be taken for different rain storms in the same day. Whenever a storm lasts longer than the end of the day, two or even more days had to be combined. The evapotranspiration input was calculated based on the hourly temperature measurements at Uccle station. Two years were selected for calibration, while the other years were used for model validation. The use of GIS in hydrology evolved along with the growing popularity of GIS in general.

Where GIS was mainly used as hydrological mapping tools in the early days, nowadays it plays an increasingly important role in hydrological modeling studies [39]. GIS can play an important role in the preparation of model input such as extracting land use and soil type characteristics for different zones in the study area. Catchment characteristics such as size, shape, slope, land use and soil type are important in shaping its runoff response. They were therefore analysed for the different calibrated catchments as follows:

- Size (area) of the catchment, and river slope (average slope between 10% and 85% of river length [173])
- Shape of the catchment
- Soil types are classified to three different groups: Sandy, Loamy, and Clayey combined with well, medium and poor drainage conditions.
- Land use characteristics are classified to three different groups: Urban area (Artificial surfaces), Agricultural areas, and Forest and semi natural areas.

For each group of soil type and land use characteristics, the sub-catchment area belonging to each of them is calculated as a percentage of the total sub-catchment area. A comparison is then made between these catchment characteristics and runoff properties. Both runoff properties directly derived from the discharge time series and NAM model parameters were considered. The NAM parameters can be considered as indirect runoff properties. To separate overland flow, interflow and baseflow properties from the time series, a numerical filtering technique was applied [178, 8]. The filter and NAM results were analyzed for two different groups: the recession constants and the water balance parameters. It can be concluded that by making use of the filter results in the NAM calibration, this calibration can be performed in a much more efficient way. The parameter values will be much more physically realistic. It will help in solving the modeling problem of finding a unique set of model parameters, which is encountered very often in the modeling practice. Based on the correlation analysis above, physically founded assumptions could be made for the NAM parameters of the ungauged sub-catchments in the Dender watershed. Furthermore, a sensitivity analysis has been performed for the rainfall input to the model. Rainfall stations located at various distances from each sub-catchment with different measuring frequencies and accuracies were available in and around the Dender watershed. Three stations with hourly rainfall data were available. The two stations of the Royal Meteorological Institute of Belgium at Uccle (30 km away from the catchment) and Melle (15 km away from the catchment) have a high measuring accuracy, while the measurements of the tippingbucket rain gauge at Elst are of lower quality. The hourly series of all these stations was used as model input, either not corrected or corrected for the rainfall volumes estimated on the basis of the daily rainfall measurements at three stations close to the catchment. This gives different types of rainfall input, for which the influence on the model results is summarized. The comparison was performed on the basis of the root mean squared difference between the simulated and observed discharges of both hydrograph peak maxima and rain storm

event minima. For this analysis, independent values have been extracted from the time series. A BoxCox transformation was applied to summarize the model accuracy in the most accurate and efficient statistical way.

A new look at hydrologic data for improving derived flood frequency parameterisations

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Understanding the physical processes giving rise to floods of a given probability of occurrence is among the most intriguing areas of catchment-scale hydrology. Not only are these processes complex and controlled by a range of variables including rainfall regime, snowmelt, state of the catchment and catchment characteristics but also their interaction is intricate. In ungauged catchments the main obstacle to realistic modeling is a lack of data that are relevant to flood processes. While catchment attributes have been used in the past as surrogates, they usually contain very little information on the actual flood processes.

In this paper we propose an alternative approach to incorporating data into hydrological models. The methodology consists of two main steps. The first step is a process classification/identification, where we identify the spatial patterns of the most important processes related to flood probabilities. We are using data that traditionally have not been used for flood frequency analyses. Most of the data we use are related to the physical unit of time (such as the time of concentration and the storm duration) which tends to be a more efficient measure of the dynamics of environmental systems than lengths and velocities. We combine different data types (multi-response data) which is based on an interpretation of typical phenomenological characteristics of hydrological processes such as periodicity. While a single characteristic may not be a unique fingerprint of that process, a combination of different sources of information is likely to much better allow the identification of processes. The classification approach has been inspired by [125] who proposed a methodology for process classification in research catchments. While no complete physical understanding of the processes is obtained by this approach, it does allow inference of the dominant process types. We derive the criteria for the classification in an iterative procedure.

In a second step we develop a modeling approach based on process types. To cope with the dilemma, that a simple model cannot describe all the flood processes (and hence cannot be used for extrapolation purposes) and more complex models suffer from the parameter estimation problem, we use a combination of simple models with different model structures and/or parameters, each model representing flood behaviour where one particular process type (as identified in the first step) is dominant. This generic approach is successfully used in a number of other disciplines where a complete physical understanding of the processes and their interaction can not be achieved due to process complexity and data limitations. One example are hydrodynamic mixing analyses that are based on a flow-classification scheme using hydrodynamic criteria to distinguish among many hydrodynamic flow pat-

terns, and very simple models for each of the classes, some of them with quite different input data [84]. As in some catchments the dominating flood mechanisms change from event to event we combine the results from the different models by applying weights representing the probability that a flood is due to one particular process. These weights are found by analysing the driving flood processes for individual events in the first step. We term this combination procedure 'process mixing' as it is based on the concept of mixed distributions. It is simple enough to allow parameter estimation for ungauged catchments and yet is detailed enough to represent the most important processes leading to floods at the catchment-scale.

Appropriate river basin modeling to assess the impact of climate change on river flooding

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How good should a river basin model be to assess the impact of climate change on river flooding for a specific geographical area? The determination of such an appropriate model should reveal which physical processes should be incorporated and which data and mathematical process descriptions should be used at which spatial and temporal scales. It should be based on sensitivities and a right balance between uncertainties of inputs, parameters and process descriptions resulting in an output uncertainty acceptable for the model user and feasible in view of data availability and computational possibilities. A procedure for determining an appropriate model is explained and applied to the above mentioned specific case. The results obtained with the appropriate model are compared with observations, results obtained with a simpler and a more complex model and uncertainties in the results. The model appropriateness procedure consists of three steps. First, the processes of importance for the specific problem are identified through a time series analysis of relevant input and output variables. These identified processes are translated to key variables by means of a qualitative analysis. In the second step, a (geo)statistical analysis with respect to these key (or indicator) variables results in appropriate spatial and temporal scales for each key variable and key variable scale-output variable relationships. These latter relationships are used to combine the appropriate spatial and temporal scales to one appropriate spatial and temporal model scale. In the third step, mathematical process descriptions consistent with these model scales are selected and used in the model. The procedure is applied to construct a model for the river Meuse basin in Western Europe to assess the impact of climate change on river flooding. Precipitation and discharge times series are used in the first step of the analysis. In the second step, ground-based and modelled climate data (precipitation, temperature) and ground-based and remotely sensed river basin data (land use, topography, soils etc.) are utilised. Moreover, a preliminary scale analysis gives additional directives for the derivation of appropriate scales. The resulting model scale is used in an existing modeling framework (IHMS) and therefore a limited number of process descriptions consistent with model scale is available. Besides the appropriate model, two additional models (a simpler one and a more complex one) are constructed to assess the sensitivity of the results to model complexity. The three models and observed rainfall input are used to simulate discharge series and derive extreme value distributions (EVDs). Comparison with the corresponding observed EVD reveals the goodness-of-fit of the models. Next, a stochastic rainfall model generates rainfall input for the current and changed climate. These rainfall inputs are used in the three river basin models to simulate discharge series and derive EVDs for the different climates. These EVDs are compared to assess the sensitivity of the results to model complexity. Finally, the uncertainty in the derived EVDs with respect to the most important inputs and parameters in the appropriate

model is estimated and compared with the results from the other two models to assess the significance of the model results as a function of model complexity. The preliminary scale analysis showed that relative large spatial scales for a few important processes were appropriate to simulate extreme discharges in an acceptable way. In accordance with this, large spatial correlation lengths from the climate data analysis seem to support relative large spatial scales. As expected the river basin analysis revealed different appropriate scales for the key variables. Peak discharge appeared to be highly dependent on precipitation and elevation resolutions and less dependent on land use and soil resolutions. Therefore, the former resolutions determine to a large extent the final model resolution. The climate data analysis showed large errors and uncertainties in RCM and GCM simulated (extreme) precipitation although corrected for averaging effects. Relative coarse spatial resolutions of the river basin data as compared to the appropriate scales do not appear to be dominant uncertainty sources.

Entropy as a sustainability indicator of agricultural practice in a river catchment

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There are many examples in the literature where the thermodynamic parameter, entropy, is used as an indicator of sustainability [2] [156]. All biotic and abiotic processes in our environment require energy and the conversion of energy from one form into another. The first law of thermodynamics states that all energy forms entering an energy-conversion process must balance the amount of energy, regardless of form, resulting from the process. The second thermodynamic law states that not all converted forms are useful to do further work (e.g. dissipated heat into the environment). This accumulation of non-useful energy is captured in the parameter termed entropy. This concept may also be applied to ecosystems where the conversion of energy for production (e.g. photosynthesis, nutrient uptake) and decomposition (e.g. biomass degradation, mineralisation) all emit by-products of energy forms that cannot be used for further work or energy conversion (e.g. respiration). This production of system-internal entropy must be compensated by the entropy of exchange processes between the system and the environment. The climax of the ecosystem corresponds to a dynamic equilibrium (steady-state), when the entropy production inside a system is balanced by the entropy flow from the system to its environment [155]. The excess amount of entropy (i.e. internal entropy production is greater than its flow from the system to the environment) reacts negatively in forms such as environmental degradation (e.g. soil erosion) and is indicative of non-sustainability.This concept is applied to an agricultural area in Saxony-Anhalt, Germany. Entropy calculations are based on life-cycle analyses of farms in a 3000 hectare region. The approach builds on the work of [151], who also applied a life-cycle analysis on an agriculturally-based lake watershed (land area = 3.3 square km), where a balance of artificial energy inputs, both mechanical (e.g. fuel and machinery) and chemical (e.g. fertilisers and pesticides), and output (yield). However, several energy forms did not enter the calculation, such as legumes nitrogen fixation, which are important energy converters. The paper also describes the methodology of upscaling these results to the river basin scale, and points to the advantages and disadvantages of using entropy for such a task compared to other indicators used for upscaling. The work will also extend the methodology to include hydrology [136] [144] and soil degradation [154].

Behavior of a hillslope-storage Boussinesq model for subsurface stormflow and saturation overland flow

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Simple but physically realistic models capable of representing hydrological processes at the catchment scale are needed for reliable simulation of overland and subsurface flow. Such models should be able to handle the spatial and temporal variability of the atmospheric, topographic, and geomorphologic characteristics that exert such an important control on the dynamics of soil moisture and groundwater and on the timing and magnitude of surface runoff generation. At the smaller scale of a hillslope the model should compare favorably against well-known physically-based models (Richards, kinematic, and Boussinesq equations, for example) under conditions where such models are known to be valid, but it should also be readily extendable to the larger catchment scale without incurring the data, mathematical, and computational complexities associated with these detailed models. For instance, large scale application of a 3D finite element Richards equation model encounters parameterization difficulties (lack of data) and high turnaround times for simulations if a fine spatio-temporal grid is needed to accurately capture rainfall-runoff transformations or to avoid numerical convergence problems. Likewise the many hillslope drainage models based on Dupuit-Forchheimer and Boussinesq theory provide convenient analytical solutions but that are not easily adaptable beyond a restricted base of assumptions (1D, homogeneous parameters, simple boundary conditions, etc). As a final requisite, these new models should be amenable to data assimilation so that they can make the best use possible of new sources for hydrological observation data. In this regard the models should be based on rigorous conservation equations and formulated in terms of meaningful (observable) state variables and parameters.

In this paper we will analyze, with regards to the criteria described above, the structure and behavior of a model recently developed by [161]. The model is based on a reformulation of Boussinesq's equation in terms of hillslope storage instead of water table height and on the method proposed by Fan and Bras [55] for collapsing a three-dimensional soil mantle into a storage capacity profile. The model implicitly accounts for a hillslope's plan curvature through the width function and for its profile curvature through the soil depth function (accounting for both terrain and bedrock shape). The result is a simple quasi-3D hillslope-storage Boussinesq model that allows for the computation of subsurface flow and saturation excess overland flow. The model is solved numerically and can handle spatially and temporally variable parameters (recharge, conductivity, boundary conditions). On the premise that a catchment is composed of 3D hillslopes with given plan and profile curvature, it should be possible to use the model as a basis for a self-consistent and efficient catchment scale model.

Comparative simulations with a 3D Richards equation-based finite element model will examine the behavior of the hillslope-storage Boussinesq model under general conditions and for special cases. In the general scenarios the spatial patterns in storage and saturation response and the outflow hydrographs will be compared for hillslopes with varying geometry and hydraulic properties. The special cases include a family of width functions for which the new model can be simplified (the influence of higher order terms in the model will be assessed), and an analysis of topographic controls via the characteristic response functions for nine basic hillslope types. The nine hillslope types are obtained by combining three plan curvatures (convergent, uniform, divergent) and three profile curvatures (concave, straight, convex).

Data Assimilation in Landscape to Model Space Mapping: the case of hydro-geochemical modeling

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The problem of equifinality in environmental modeling means that the prediction process might be best posed as an uncertain or fuzzy landscape space to model space mapping. This results in an approach to hypothesis testing and data assimilation that is concerned with refining the set of feasible models within the model space and, in particular, rejecting some of those models where additional data suggest that they are no longer adequate. This is explored here within the context of catchment scale rainfall-runoff modeling, together with the additional dimensions in model space added by geochemical modeling components. Particular attention is paid to effective mixing volume parameters that are often assumed to be the same for predicting both discharges and concentrations at the catchment scale. Physically, there is no reason why these should be the same and the value of different types of data in constraining the feasible values is explored.

2 Data assimilation methods
Chairman: J. Grasman

Data assimilation methods in meteorology and oceanography

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The purpose of data assimilation is to produce as accurate as possible a description of the state of the system under observation, using all the available relevant information. In environmental science applications, the available information usually consists of observations proper, nd of the physical laws governing the system. The latter are available in the form of a discretized, necessarily approximate, and usually large-dimensional numerical model. The large numerical dimension of the problem is one of the major sources of difficulty in environmental applications of assimilation. Two main classes of algorithms are used in meteorology and oceanography. Sequential assimilation, of which Kalman filtering is the theoretically optimal form in linear cases, constantly updates the latest state estimate by using new observations. It requires in principle the explicit computation of the temporal evolution of the uncertainty on the current state estimate. This requirement substantially loadens the computational cost of sequential estimation. The definition of methods for explicitly computing the temporal evolution of the uncertainty, while being both accurate enough for being useful and economical enough for being practically implementable, is the subject of active research. Sequential assimilation can relatively easily take the model error into account, by an appropriate inflation of the growth of the state estimate uncertainty. On the other hand, it carries information only from the past into the future. This is not desirable if one wants to assimilate past data, for instance for climatic purposes. Kalman filtering can in principle be extended to backward assimilation in the form of Kalman smoothing. Kalman smoothing has however not been studied very much so far in meteorological and oceanographical applications. Variational assimilation, on the other hand, globally adjusts the assimilating model to observations distributed in time. This is achieved through minimization of an 'objective function' measuring the misfit between the model and the observations. The minimization is made numerically possible through the use of the adjoint of the assimilating model. Variational assimilation propagates information both forward and backward in time. The fact that it produces, at a non-prohibitive cost, fields that are consistent with the model dynamics is the major reason why variational assimilation is more and more used for operational numerical weather prediction. On the negative side, variational assimilation does not easily produce an estimate of the uncertainty on the assimilated fields.

Variational assimilation, as it is implemented at present, imposes the model equations as a 'strong constraint' to be exactly verified by the assimilated fields. This becomes a distinctive drawback for longer assimilation periods. 'Weak constraint' assimilation, in which the model error can be taken into account (provided it has previously been quantified), is in principle possible. The so-called 'dual' algorithm seems in this respect to be very promising. The development of weak constraint variational algorithms is still however at a rather early stage.

All those various algorithms, in the linear case, solve the same least-squares estimation problem (either with or without model error, depending on the particular algorithm under consideration). It is only when an appropriate linear approximation is valid that they can be confidently used, and that precise statements can be made as to the properties of the assimilated fields. Assimilation methods must always be assessed with respect to the degree of linearity of the assimilating model. In the case of a strongly nonlinear model, it may be that the best way to perform assimilation is ensemble assimilation, which does not produce one estimate of the state of the system, but a number of estimates, whose dispersion is meant to represent the corresponding uncertainty.

An inter-comparison of cross-validation and Kalman filtering algorithms

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The monte-carlo approach to Kalman Filtering has proven to be successful. Over the past decade the ensemble Kalman filter was conceived and applied [24, 49, 52, 77]. Another approach to reduce the computational burden of the Kalman filter, is via a reduced-rank version of the square root filter, [169, 170]. Recently, the integration of the two methods has been realized and shown to be efficient [74]. In spite of the computational efficiency of these filters when compared to the full Kalman filter, they are are still demanding. In addition it is still unclear how they compare more simple methods for recursive state estimation. In this study a sophisticated variant of the ensemble Kalman filter (COFFEE, as described in [74]) are compared to a relatively simple filtering approach which is based on cross-validation [166]. The cross-validation filter uses information about the efficiency of various observations to update the gain matrix directly, i.e. without first estimating the model covariance. The information about the efficiency of various observations is obtained by repeatedly dropping an observation and determining the effect of this on the state estimation at the next time instant where observations become available. The cross-validation filter is especially useful if observations are available relatively infrequent, or if the model error is relatively large or unknown [166].

The filters are tested on a catchment-scale soil-moisture prediction problem where discharge, ground water as well as soil moisture observations are assimilated in a distributed model. The model is defined on a 20×20 m grid and comprises a 2D subsurface and 1D surface component. 3/4th of the observations are used for assimilation and 1/4th are used for validation purposes. In particular, the filters are compared with an open-loop simulation, a case where all available data are used (*data-rich*) for assimilation and a case where only the ground water and discharge data are used (*data-poor*). As expected, data assimilation always improves the soil-moisture predictions considerably. The relatively good performance of the data-poor case is a little surprising. It turns out that both filters perform similar, but when looking in detail the cross-validation outperforms COFFEE in the data-poor cases and in cases with low-soil moisture content. It appears that in these situations the observation error is relatively large. This effect has not been taken into account in COFFEE as implemented here, and is automatically considered by the cross-validation filter.

Optimisation of a piezometer network using a statistical space-time model and the Kalman filter

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Water authorities in The Netherlands are not only responsible for managing surface water, but also for managing the groundwater reserves. Particularly the water table depth is an important variable, determining agricultural production and the potential for nature development. Knowledge of the spatio-temporal variation of the water table depth is therefore vitally important for regional scale water management. This raises the following question: At what spatial density and which temporal frequency must the water table depth be observed to obtain a complete spatio-temporal picture at a required accuracy and at minimal costs. In this paper this problem is tackled by using a statistical space-time model of the water table depth in combination with a space-time Kalman filter.

The statistical model is built as follows. A simple time series model (called ARX model) is used to describe water table depth as a function of precipitation surplus (precipitation minus potential evapotranspiration). The ARX model is calibrated first at locations where time series of water table depth are available [17]. ARX parameters at non-visited locations are estimated through geostatistical interpolation using auxiliary information, such as surface elevation from a digital elevation model (DEM). The result is a so called regionalized ARX model or RARX model [88]. The parameters of the geostatistical model (i.e. the semi-variogram) are estimated by embedding the RARX model in a space-time Kalman filter and minimisation of a maximum likelihood criterion built from the filter innovations. The resulting state-space model can be used for optimal space-time prediction of water table depth, space-time conditional simulation and network optimisation [16]. The parameters of the RARX model can interpreted physically, such that the predicted water table depth can used to predict specific drainage discharge. Hence, it is possible to predict the total discharge from a catchment with predominantly groundwater flow. This way, it is also possible to assimilate discharge measurements to improve predictions of water table depth.

A case study is presented where the RARX model and the Kalman filter are used for optimisation of an existing network of 233 piezometers in the water authority Reest and Wieden, The Netherlands. Water table depths are recorded two times a month for all locations. Observation and maintenance costs of this network are high. The accuracy of the existing network is analysed using the RARX model and the Kalman filter. The accuracy is both "modelled" (assuming an additive noise process that is discrete and white in time and continuous, coloured and multi-Gaussian in space) and estimated with cross-validation. Several options for decreasing observation efforts are analysed. A particularly promising option is observing a limited number of well placed locations with high frequency (i.e. using divers) and the remaining locations only occasionally.

Estimation of model error covariance matrices for different land-atmosphere hydrology models

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The model error covariance matrix Q is an often unknown, yet necessary parameter for the implementation of Kalman filtering. In the hydrologic data assimilation context Q is a measure of how much forcing noise needs to be included in the hydrology model used. While the measurement error covariance matrix R can in general be determined from instrument characteristics, there is little guidance for most hydrologic models as to how what value should be given for Q, or even how to model this error. In this work, we present the values of Q for several land-atmosphere hydrologic models, in which the state variables are soil moisture and temperature and canopy (intercepted) moisture. Precipitation and net radiation are used as forcing variables, while the desirability of using measured land surface energy fluxes as state variables is explored. The Q matrices are derived by applying maximum likelihood estimation techniques to the extended Kalman filter methodology of data assimilation, minimizing the residuals between the ideal (unknown) state variables and their filter estimates. Land surface measurements of micro-meteorologic variables and energy fluxes taken during the Southern Great Plains 99 (SGP99) experiment are used to drive the estimation. By explicitly calculating the model error covariance structure of different land-atmosphere hydrology models for a given set of environmental measurements, choices about which model may be appropriate for use in a data-assimilation framework can be clarified.

A VFSA (Very Fast Simulated Annealing) Approach for Land Surface Data Assimilation

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The high nonlinearity and discontinuity of land-surface model and radiative transfer model (used as the observation operator) hinder further practical operation of some advanced 4DDA (four dimensional data assimilation) methods such as the Kalman filter and the variational method in the land-surface data assimilation system. The Kalman filter or the extended Kalman filter needs a linear or quasi-linear model; and the variational method needs an adjoint model for minimization, which can not handle the discontinuity resulted from including thresholds in the land surface model [110]. Therefore, the Kalman filter and the variational method, when applied to land surface data assimilation, usually need simplified or linearized model operators and observation operators. Evidently, simplification and linearization, if not impossible for a fully coupled system, sometimes result in the inconsistency of the cost function and its gradient. Moreover, many physical details of the original model operator and observation operator are lost. Accordingly, We develop a new data assimilation algorithm by employing a heuristic optimization approach named simulated annealing [87, 129], which is capable to minimize the four dimensional cost function without using the adjoint model. The method has advantages in dealing with the strong nonlinearity and discontinuity, and in finding the global minimal in the hilly structure of the cost function [9, 50, 95]. Additionally, all the processes in the model operator and the observation operator can be kept because the method is independent on the cost function. The disadvantage of this method, when compared to the variational method, is its low efficiency. Therefore, we make efforts to improve the method by incorporating very fast simulated annealing (VFSA) and re-annealing algorithms [80, 157] into the data assimilation cycle. Based on the VFSA algorithm, we design a research-operational land surface data assimilation system which can assimilate both the in situ monitoring of soil moisture and soil temperature, and the passive microwave remote sensing observations into a land surface scheme. The modified SiB2 with frozen soil parameterization [101] is used as the model operator, and the radiative transfer model of moist soil [89]is used as the observation operator to transfer the brightness temperature into model variables of soil moisture and surface temperature. The performance of the algorithm mainly depends on the annealing schedule and the generator of random changes of state vector. In VFSA, the annealing approach is an analogy with thermodynamics, specially with the way that metals cool and anneal. The annealing procedures can be described as: The state vector is constrained by

$$x \in [R_l, R_h]$$

where, $x = [\theta_1, \theta_2, \theta_3, T_g]^T$ is a vector of soil moisture profile (θ_1, soil moisture of the surface layer; θ_2, soil moisture of the root zone; θ_3, soil moisture of recharge zone) and surface temperature T_g; R_l and R_h are two N dimensional vectors of low and high range of x. x is updated with a random increment δx,

$$x_{i+1} = x + \delta x(R_h + R_l)$$

where the subscript i is the time of iteration in minimization.

The element of δx is generated from a $\underline{u}$ from the uniform distribution

$$u^j \in U[0,1]$$
$$\delta x^j = sgn(u^j - \tfrac{1}{2})T^j \left[\left(1 + \tfrac{1}{T^j}\right)^{|2u^j - 1|} - 1 \right]$$

where, j is the jth element of a N dimensional vector. The annealing schedule for T is

$$T_i = T_0 exp(-ci^{1/N})$$

where, N is the dimension of the assimilating state vector; c is an analogy to the "Boltzmann's constant" . We have implemented one dimensional offline test of the algorithm with the GAME-Tibet observations. The algorithm is compared with a control run without assimilating the observations. The results show that the cost value calculated from the optimized initial values is much smaller. In addition, the bias from observations is also significantly reduced. We are going to make the in situ and two dimensional test with SSM/I and TMI observations.

A Coupled Land Surface-Boundary Layer Model and Its Adjoint

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In meteorology and oceanography there is a well-established history of using variational techniques for sensitivity analysis as well as data assimilation (e.g. [97], [120], [158]). This is due in large part to the nature of many research problems in these fields. Often, large state, parameter, and forcing fields and/or extensive datasets of meteorological measurements require an efficient technique to evaluate sensitivities required for sensitivity analysis or data assimilation. Adjoint models can be ideal tools in such circumstances due to their relative computational efficiency in comparison to simulation techniques. Recently, adjoint models have begun to be used in surface hydrology applications (e.g. [25], [138], [19], and [137]), especially in data assimilation. This is in large part due to the fact that hydrology has gone from a somewhat "data poor" to a "data rich" environment as hydrologic data have become much more prevalent with the increase in remote sensing capabilities. With the advent of large datasets and complex models, many of the issues that led meteorologists and oceanographers to use adjoint techniques are now at the forefront in hydrology.

The overall objective of this research is to design a framework for the statistically optimal assimilation of observations into a coupled land surface-boundary layer model. The adjoint model is derived from a forward model of the coupled land-atmosphere system and can be used in a variational data assimilation framework to yield dynamically consistent estimates of land surface states and fluxes which optimally combine observations with the model of the physical system. The model and its adjoint can also be used for sensitivity analysis that are more insightful and efficient than simple perturbation-simulation approaches.

Land Surface-Boundary Layer Model

The model we have developed for use in this study is composed of a detailed land surface model, and an accompanying mixed-layer model representation of the overlying boundary layer. The description of the model and its testing is presented in detail in [109].

The core of the model involves solving the coupled energy and water budget equations of the land surface and overlying atmospheric boundary layer. The land surface component of the model consists of prognostic equations for three temperature states (canopy temperature, surface ground temperature, and deep ground temperature) and three soil moisture states representing the soil moisture profile through the uppermost 1-2 meters of soil. For the boundary layer we use a mixed-layer model. The model includes a parameterization of the daytime growth and evening collapse of the mixed-layer. Entrainment fluxes which occur in conjunction with the ABL growth (and generally bring warm/dry air down into the mixed layer) are also included. In addition, a parameterization of the radiative feedback

between the surface and overlying atmosphere is included in the model. Thus our model, while remaining relatively simple, includes most of the primary interaction pathways in the land surface-ABL system. Finally, by simultaneously taking into account the coupled nature of the system, the forcing requirements for the model are reduced to only incoming solar radiation, large-scale wind speed, and lapse rates in temperature and humidity above the mixed-layer. We are thus able to model the system with a minimal set of auxiliary data.

Adjoint Model Development and Validation

The development of the adjoint model is relatively straightforward, and is described in detail in [109]. While straightforward, the process involves multiple applications of the chain rule which can be both tedious and error prone. Therefore, using some simple tests, the validity of the adjoint model was heavily tested before applying it to any data assimilation problems [109].

A Simple Data Assimilation Example

The primary benefit of choosing a variational data assimilation approach is that it can efficiently yield dynamically consistent estimates of land surface states and fluxes which optimally combine observations with the model of the physical system. In order to illustrate this, we chose a simple synthetic initialization problem in which our objective was to estimate the model initial conditions which minimize the model-measurement misfit.

For the synthetic problem, the imperfect measurements to be assimilated were of ground temperature. We wished to minimize a least-squares objective function, which included a penalty term for the model-measurement misfit and a prior term. The two error covariances related to these terms weight the model-measurement misfit and prior estimate misfit respectively based on the uncertainty involved in each component. Once the adjoint model is integrated backward in time, the gradient of the objective function with respect to the initial conditions can be computed and used in a gradient search to find the optimal initial condition estimates. This procedure is repeated iteratively until convergence is reached. Having obtained optimal estimates of the initial conditions, dynamically consistent optimal estimates of the model states and fluxes are obtained via a forward model integration.

Results from this simple example illustrate that the algorithm not only ultimately fits the temperature state to the measurements quite well, but that through the model dynamics other states (for which there are no assimilated measurements) are also updated, removing strong biases ($\sim 1-5$ K in the temperature states; $\sim 1-2$ g kg^{-1} in specific humidity; and $\sim 10-20\%$ in soil moisture) that were present based on the prior parameter values. Also, we are often most interested in estimating the fluxes between the land surface and atmosphere which constitute the surface energy balance. The estimates based on the prior values underestimated peak sensible heat flux by ~ 20 Wm^{-2} and overestimated peak latent heat flux by ~ 40 Wm^{-2}, while also having a large bias throughout the day. In contrast, the sensible and latent heat flux values from the estimated parameters almost exactly reproduce the actual values throughout the day. Thus the results overwhelmingly

show that the assimilation of data greatly improves our ability to predict all of the states and fluxes at the land surface.

Ongoing Research

Ongoing research efforts include applying the framework described above to other problems. This includes investigating the ability of assimilation of ground temperature at the FIFE site to estimate other surface states and the surface turbulent fluxes. Specific research questions include: how often measurements are required to produce accurate estimates, at what intervals, time-of-day etc. This would not only be relevant for sites with in-situ ground temperature measurements, but potentially for sites monitored remotely with thermal infra-red satellites. Another topic being investigated is the potential use of micrometeorological data (air temperature and specific humidity) as assimilated variables. In contrast to other variables, this data is often readily available at high temporal resolution (i.e. 30 minute micrometeorological station measurements). While many models require this data as forcing, our coupled model does not, and therefore the additional information contained in this readily available data may allow for the estimation of other unknown states and fluxes. In addition to these research questions, the framework described above is sufficiently general that it could be applied to other relevant problems in the future.

Using representers for inverse modeling of groundwater flow and transport

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It needs no introduction that efficient and reliable spatially distributed groundwater flow and transport models are essential for the prediction and evaluation of groundwater pollution. The modeling process consists of two steps. The first step is the groundwater flow model, describing the behaviour of groundwater heads and velocities as a response to driving forces. These driving forces maybe precipitation, surface water, groundwater abstraction etc. The relation between the driving forces and the heads and velocities are determined by flow parameters, such as permeability and storativity. The second step is the transport model. In this model the concentration is described as response to the chemical driving forces, which are the sources of the pollutant. The transport model contains chemical parameters, such as sorption and retardation. The groundwater flow field acts in the transport model as a parameter.

The parameters and driving forces are uncertain. Moreover, models are always a simplification of reality. The imperfectness of the models introduces a model errors. Because of the model errors and the uncertainties in parameters and driving forces the predicted concentrations differ from the reality. To eliminate or minimise the error in the resulting concentrations measurements of the state variables are taken. This can be measurements of the groundwater head, groundwater concentration or soil concentration. The measurements are used in an inverse modeling approach to decrease the uncertainty of the input parameters and the model error and consequently the error of the predicted concentrations will be decreased. In the inverse modeling approach an objective function is used that accounts for measurement errors and parameter uncertainty as well as for model errors.

In groundwater flow and transport problems, this type of inverse modeling is very complex as the number of unknowns parameters and model errors becomes very large in three-dimensional real world problems. The current inverse approaches need too much calculation time and/or data storage to solve this type of problems. In this poster an inverse approach is introduced that reduces the amount of computation time and data storage considerably. It uses an optimal parameterisation by introducing representer functions for all measurements. Representer functions show the influence of a single measurement on the parameters and the state variables (heads, velocities and concentrations) that are to be estimated. The representer functions show the adjustment of the parameters and state variables due to a unit misfit between the measurement and the corresponding model prediction. The magnitude of the adjustment depends on the magnitude of the misfit. The

number of independent estimation parameters reduces to the number of measurements. This type of parameterisation is optimal in the sense that the final result is equal to the solution of the full-scale inverse problem. It provides also estimates of the posterior uncertainty of both parameters and state variables.

The method is tested on two synthetic examples where controlled experiments were performed. In these examples the relative improvement due to measurements of the head, mobile concentration and immobile concentration are analysed. Some results of the application in a real world case will be presented.

The method of representer functions appears to be attractive for parameter and state estimation. It allows inverse modeling of large real world cases, provided that the number of measurements is small. Almost all 3-dimensional groundwater flow and transport models have large amounts of grid nodes. However, the number of available measurements is normally orders of magnitude smaller than the number of grid nodes. Therefore, the method of representer functions is applicable is many real world cases. In addition to estimate of parameters and state variables also the corresponding uncertainty is quantified.

A very promising application of the representer function method is in designing monitoring strategies. The representer functions visualise explicitely the amount of information that an individual measurement contains for the estimation of parameters and state variables. One measurement may contain much information for estimation of a state variable, whereas at the same time it might not contribute significantly to the estimation of a particular parameter. The explicit form of the information contents allows judging the effectiveness of actual and future monitoring schemes. Moreover, the relative impact of measurements of different variables can be compared. Particularly interesting is the analysis of the impact of monitoring schemes with combinations of head and concentration measurements.

Automatic differentiation and model uncertainty analysis

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In the talk we compare the automatic differentiation approach to methods traditionally used for model calibration of large models, such as the adjoint method. We further discuss how AD can be used to investigate several types of modeling uncertainty. The main emphasis will be on sensitivity analysis, parameter estimation uncertainty and the optimal choice of model complexity. For the parameter uncertainty estimation we will consider the influence of model nonlinearity on the quality of the parameter estimates.

Kalman filtering algorithms for data assimilation in large scale transport models

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Kalman filtering is a powerful framework for solving data assimilation problems (see [68]). In order to use a Kalman filter for assimilating data into a numerical model, this model is embedded into a stochastic environment by introducing a system noise process. In this way it is possible to take into account the inaccuracies of the underlying deterministic system. By using a Kalman filter, the information provided by the resulting stochastic-dynamic model and the noisy measurements are combined to obtain an optimal estimate of the state of the system. The standard Kalman filter implementation however would impose an unacceptable computational burden. In order to obtain a computationally efficient filter simplifications have to be introduced.

The Ensemble Kalman filter (EnKF) was introduced by [49] and has been used successfully in many applications (see [24, 52, 77]). This Monte Carlo approach is based on a representation of the probability density of the state estimate by a finite number N of randomly generated system states. The algorithm does not require a tangent linear model and is very easy to implement. The computational effort required for the EnKF is approximately N times as much as the effort required for the underlying model. The only serious disadvantage is that the statistical error in the estimates of the mean and covariance matrix from a sample decreases very slowly for larger sample size. This is a well known fundamental problem with all Monte Carlo methods. As a result for most practical problems the sample size has to be chosen rather large.

Another approach to solve large scale Kalman filtering problems is to approximate the full covariance matrix of the state estimate by a matrix with reduced rank. This approach was introduced by [32, 33] and [169, 170] where the latter used a robust square root formulation for the filter implementation. Algorithms based on similar ideas have been proposed and applied by [100, 127].

The reduced-rank approaches can also be formulated as an Ensemble Kalman filter where the q ensemble members have not been chosen randomly, but in the directions of the q leading eigenvectors of the covariance matrix (see [170]). As a result also these algorithms do not require a tangent linear model. The computational effort required is approximately $q+1$ model simulations plus the computations required for the singular value decomposition to determine the leading eigenvectors $O(q^3)$, see [73]. In many practical problems the full covariance can be approximated accurately by a reduced-rank matrix with relatively small value of q. However, reduced-rank approaches often suffer from filter divergence problems for small values of q. This was observed first by [32], who tried several methods of compensating for the truncation error. The main reason for the occurrence of filter divergence is the fact that truncation of the eigenvectors of the covariance matrix implies

that the covariance is always underestimated. It is well-known that underestimating the covariance may cause filter divergence. Filter divergence can be avoided by choosing q relatively large, but this of course reduces the computational efficiency of the method considerably.

Very recently [74] propose to combine the EnKF with the reduced-rank approach to reduce the statistical error of the ensemble filter. This is known as variance reduction, referring to the variance of the statistical error of the ensemble approach (see [72]). The ensemble of the new filter algorithm now consists of two parts: q ensembles in the direction of the q leading eigenvalues of the covariance matrix and n randomly chosen ensembles. In the algorithm, only the projection of the random ensemble members orthogonal to the first ensemble members is used to obtain the state estimate. This Partially Orthogonal Ensemble Kalman filter (POEnKF) does not suffer from divergence problems because the reduced-rank approximation is embedded in an EnKF. The EnKF acts as a compensating mechanism for the truncation error. At the same time POEnKF is more accurate than the ensemble filter with ensemble size $N+q$ because the leading eigenvectors of the covariance matrix are computed accurately using the full (extended) Kalman filter equations without statistical errors.

In our paper we first introduce the Kalman filter as a frame work for data assimilation. Then we summarize the Ensemble Kalman filter, the Reduced-Rank Square Root filter and the Partially Orthogonal Ensemble Kalman filter and a few variants of this algorithm. We finally illustrate the performance of the various algorithms with a number of different advection diffusion model applications.

3 Spatial data and distributed models
Chairman: G. Blöschl

Observed spatial patterns for developing and testing distributed models - the key to progress

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For many years now, modeling tools have been available to simulate spatially distributed hydrological processes.The quality of the simulations and spatial process representation have been difficult to assess because of a lack of appropriate data. Appropriate means that they tell us about system behaviour, test critical assumptions in our understanding and in our models of that understanding, and provide enough information to resolve the problems of non-uniqueness and parameter identifiability inherent in complex models. Observed patterns of hydrological response can be powerful in these respects.

This talk will focus on the utility of using spatial data in model development and testing and illustrate the complementarity between these data and more traditional hydrologic observations. The use of observed patterns to provide model inputs, parameter values, and for comparison with simulated spatial output, will be discussed. Examples will cover a range of model types, scales, dominant hydrological processes and include both remotely sensed and ground-based data sets. Specifically, examples of observed patterns obtained from airborne sensors include rainfall from ESTAR surface brightness temperatures, soil moisture from passive microwave data, and snow cover from aerial photographs Patterns from space borne sensors will include SAR derived soil moisture. Observed ground based patterns are even more diverse and will include water levels from a dense network of piezometers, runoff occurrence from an intensive network of runoff detectors, and soil moisture sampled on a dense regular grid. Indicator (proxy) data such as observations of long term recharge and discharge at numerous locations in a catchment will also be discussed. All of these examples clearly demonstrate that, even with quite simple comparisons, spatial patterns provide an extraordinarily rigorous test of distributed models and of our understanding of system response. For example, detailed soil moisture patterns are used to identify structural improvements required in a small-catchment model, including the need to represent the temporal dynamics of soil hydraulic properties; the use of pedotransfer functions along with soil maps is shown to result in poor simulations of spatial response in several different model applications at different scales; and the relative importance to snow distribution of representing wind and radiation is illustrated for alpine and rolling terrain. Challenges for the use of patterns in modeling will also be discussed, including the need for more quantitative pattern comparison methods; interpolation techniques that better suit hydrological applications; better use of binary or categorical patterns, and computationally tractable uncertainty techniques for use with pattern information.

Influence of Small-Scale Topography on the Hydrologic Behavior of a Catchment-Based Land Surface Model

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The realistic representation of land surface processes is critical for the realistic simulation of the global hydrologic cycle and climate, as indicated by numerous sensitivity studies using general circulation models (GCMs). Land surface-models (LSMs) have therefore increased in sophistication and realism over the last decade. Much effort has focused on the modeling of point processes (e.g. canopy structure and resistances to evaporation). As a consequence, soil moisture is assumed in most LSMs to be uniform at the GCM scale, the soil being described as a stack of vertical layers. The transfer of moisture between the layers, which has a crucial impact on both baseflow and overland flow production, is then computed one-dimensionally, along the vertical only. This is overwhelmingly unrealistic given the small scale variability of soil moisture, largely imposed by precipitation heterogeneity and the lateral redistribution of moisture following topography.

An original LSM for GCMs was recently developed by [93] to account for the effect of topography on the small-scale variability of soil moisture and its effects on runoff and evaporation. In a break from traditional approaches, this model recognizes the hydrologic catchment as the elementary land-surface unit, with boundaries that are dictated by topography instead of a regular grid. This is made possible by the recent developments at the global scale of high-resolution, hydrologically correct, digital elevation models (DEMs). The example used to constrain our catchment-based LSM is the HYDRO-1K database, derived at the USGS from the 30 arc-second DEM GTOPO30 [168]. In each catchment, the small-scale topography is characterized by the distribution of a topographic index [15]. This distribution is combined at each time step to the bulk catchment moisture to derive a root zone moisture distribution, used to separate the catchment into three areal fractions (saturated, unsaturated, stressed). These different areas have very different physics, and a key feature of the model is that evaporation and runoff are calculated independently over each one, using formulations relevant to the hydrological regime.
This LSM uses three non-traditional bulk moisture variables to describe the catchment moisture state. One represents equilibrium conditions associated with the water table distribution, which is diagnosed from the topographic index distribution using TOPMODEL's equations [15, 145]. Two additional prognostic variables represent non-equilibrium conditions in the root zone and the top centimeters of soil. Three processes in the model depend

on both topography and these prognostic variables, in a highly complex way. These are baseflow, the vertical water transfers in the unsaturated zone, and the lateral distribution of root zone moisture. An important feature of the model is that these processes are satisfactorily approximated by simple, tractable functions of the prognostic variables only [46]. Under this framework, the influence of the catchment topography is represented implicitly, by the parameters of these empirical functions. The latter are preprocessed in every unit catchment, and used at each timestep in the model, which strongly enhances its performance in terms of computing requirements.

The evaluation of such an LSM must address two separate issues: (1) does it realistically transform the atmospheric forcing into surface fluxes? and (2) does it capture the influence of topography on the surface water budget? A partial answer to the first question was given by a detailed analysis of the LSM's behavior in the Red-Arkansas River Basin. This domain of about 565,000 km^2 is subdivided into 126 unit catchments according to HYDRO-1K. In each of them, the LSM is run off-line, using the framework developed for PILPS Phase2c [181] which includes 10 years of meteorological forcing. An important advantage of this testing framework is the quality of the validation data, which consists of two independent datasets: daily streamflow (1979 to 1988) at the outlets of the two basins, and monthly total evaporation over the entire domain, estimated from 1980 to 1986 through an atmospheric budget analysis. This work showed excellent performances of the catchment-based LSM on average over 1980-1986. In addition, the LSM reproduces well the seasonal cycle and the inter-annual variability of evaporation and runoff [46].

Here, we will focus more closely on the second issue, namely the influence of topography on the hydrological behavior of the catchment-based LSM. In an idealized experiment, we forced the 5020 catchments composing North-America in HYDRO-1K with the same forcing data for vegetation, soil and meteorological conditions. Thus, the only differences between the catchments are their topography. This exercise showed variations between the catchments that reached 15% for annual mean evaporation and 20% for annual runoff [46]. This demonstrates the importance of small-scale topographical heterogeneity with respect to the simulated fluxes.
In particular, the shape of the topographic index distribution is known to be altered by the resolution of the DEM used to compute the topographic indices [180]. The influence of the DEM's resolution on the simulated water and energy budgets will be studied in the Seine river basin (France). The catchment-based LSM has already been applied with satisfying results in this 75,000-km^2 basin (subdivided into 29 unit catchments), using a 1000-m DEM (HYDRO-1K). A100-m DEM (derived from digitized maps) has recently been acquired for comparison.

Incorporating spatial information into conceptual rainfall-runoff models using multi-criteria methods

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The "semi-distributed" approach to modeling the spatial variability of important hydrologic processes is becoming popular as the availability of high-resolution hydrologic information continues to increase. However, the spatial detail with which this variability needs to be represented to provide accurate streamflow simulations is not well understood. Further, the increased complexity of the semi-distributed approach (and in particular the large number of parameters) results in a calibration problem of considerable difficulty. Traditional manual and automatic calibration approaches typically provide a single sub-optimal solution, with little or no information about the uncertainty in the estimated parameters or the model performance. In this study, we assess the performance improvements of semi-distributed applications of the U.S. National Weather Service Sacramento Soil Moisture Accounting (SAC-SMA) model on a watershed using radar-based remotely sensed precipitation data. Specifically, performance comparisons are made within an automated multi-criteria calibration framework to evaluate the benefit of "spatial distribution" of the model input (precipitation), structural components (soil moisture and streamflow routing computations), and surface characteristics (parameters). A comparison of these results is made with those obtained through manual calibration.

Implications of non-linearity and data uncertainty for hydrological modeling

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modeling catchment response, in terms of flow and transport, is complicated by the strong non-linearities of the governing processes and the heterogeneity of natural soils. The interplay between nonlinearity and heterogeneity, often, leads to a large variability of infiltration in space and time [58] at a range of scales which is reflected in two typical flow regimes of soil water - fast preferential flow due to fingering effects or flow in macro-pores, and slow matrix flow. In principle, soil properties and state variables that favour the occurrence of preferential flow can be determined by field experiments but subtle changes in these variables can translate into major changes in hydrologic response. Lennartz et al. [99], for example, monitored the transport of surface applied Bromide for three subsequent years on a drained field site, and showed that a high susceptibility to preferential flow was an intrinsic property of the soil. In a similar study, Villholth et al. [171] identified vertical earthworm burrows as active preferential pathways, and Zehe and Flühler [187] analysed 10 plot scale irrigation experiments and showed that a higher macro-porosity apparently predisposes a field site to preferential flow. The latter study also showed that a small increase of the initial saturation S from 0.2 to 0.4 will make the system switch from matrix flow to preferential flow which suggests that threshold processes are operative. These are clearly highly non-linear.

The purpose of this study is twofold: (a) to shed light on the degree and type of non-linearity one has to expect as soils switch from matrix to preferential flow, and (b) to assess the feasibility of inferring hydrologic response from plot scale measurements given the inherent uncertainties of these measurements due to measurement error and scale incompatibility. We chose a Monte Carlo simulation approach which we conditioned by comprehensive field measurements. Specifically, we simulated the performance of repeated trials of a plot scale irrigation experiment in a heterogeneous soil over a wide range of initial saturation values and related the initial saturation to the flow regime. We generated realisations of the saturation values to reflect realistic measurement errors and the scale incompatibility of TDR-probes (100 ccm cylinders) with REVs usually used in hydrologic modeling [18].

We performed the field measurements on a 1.4 by 1.4 m^2 plot which we irrigated with tracer solution over 2 hours using a dye (Brilliant Blue) and a conservative tracer (Bromide). Tracer concentrations were measured for 0.1 by 0.1 m^2 cells. The initial saturation in the upper 0.15 m of the soil was measured on two separate plots of 4 m^2 size at 25 points using a two-rod TDR sensor. Each point measurement was repeated 5 times to estimate

the random measurement error. For these experiments, the average initial saturation and its standard deviation were estimated to be 0.62 and 0.04, respectively. Additionally, the number, widths and depths of the macro-pores were determined for two horizontal soil profiles of 4 m^2. Undisturbed samples from the soil matrix as well as macro-porous soil samples were extracted from two depths at these profiles and analysed for their porosity and saturated water flow rate in the laboratory. We used CATFLOW as the numerical modeling system which represents soil water and solute dynamics using the 2D Richards equation and a 2D transport equation of the convection - dispersion type. Water flow and transport in the macro-pores are represented by a simplified approach which assumes that if the relative saturation at the surface of a macro-porous model element exceeds a threshold S0, the bulk hydraulic conductivities of this grid point and all macro-porous grid points below are increased by the macro-porosity factor f. Macro-pore flow and matrix flow are simulated in the same domain and we defined an effective flow velocity in a model grid cell as the geometric mean of the flow velocities in the macro-pores and the soil matrix. For the Monte Carlo study a macro-porous medium was stochastically generated in two steps. First a macro-pore distribution with the observed properties was generated based on the condition that the fraction of the unit area covered by the cross-sectional area of macro-pores of a constant radius is equal to the probability of their occurrence in the field. Second the distribution of the macro-porosity factor f was generated based on the observed water flow rates in the macro-porous soil samples. The macro-porous medium and its hydraulic properties were generated once and kept constant throughout the whole study. The threshold for initiating macro-pore flow was chosen to be S0 = 0.6 which corresponds to the saturation at field capacity. As a next step, 40 different realisations of the field of initial water content with the same mean, standard deviation and spatial correlation were generated using the turning bands method [21]. These fields differ, however, in their patterns and these differences have been assumed to reflect data uncertainty. Because of these differences, the correlations between the generated field of soil hydraulic properties and the initial water content were different for each realisation which cause changes in the simulated tracer distribution. The simulation procedure was repeated for different mean initial water contents. The calculated tracer distributions were characterised by the average depth of the Bromide centre of mass in the vertical columns of the computational grid, as well as the standard deviation of the Bromide centre of mass within these columns. For an average initial saturation of 0.62 as observed in the irrigation experiment, the parameters characterising the simulated flow patterns were close to the observed values. This suggests that the model is a good representation of the flow and transport processes in the field.

The simulation study gave the following results. Average initial saturation values lower than 0.30 produced flow patterns with small average depths and small standard deviations of the Bromide centre of mass, i.e. matrix flow dominated, and there was very little variability between the results of the realisations, i.e. small changes in the inputs (average initial saturation) caused small changes in the outputs (type of the flow regime). Average initial saturation values larger than 0.53 produced flow patterns with large average depths

and large standard deviations of the Bromide centre of mass, i.e. preferential flow dominated, but there was again very little variability between the results of the realisations. We call these ranges (S<0.3; S>0.53) stable. The interplay between hydrologic non-linearity and data uncertainty is unlikely to affect catchment response very much as long as the soil moisture is within these bounds. The simulations with average initial saturation values between 0.3 and 0.53 produced a completely different behaviour. For a particular realisation, either matrix flow or preferential flow would occur randomly. We call this range unstable because, in this range, the type of flow regime will be determined by virtually unobservable details that one cannot hope to capture in a hydrologic field study.

In humid climates as examined here, the results of this study have important ramifications for hydrologic modeling at a range of scales. At small scales, one can expect large inherent uncertainties in hydrologic response when soil moisture is in the unstable intermediate range. Here, the interplay of hydrologic non-linearity and data uncertainty becomes important and threshold processes can switch between the two regimes. For both very dry and very wet soil moisture conditions one can expect relatively small predictive errors and more linear dynamics. At larger catchment scales, the effect of data uncertainty and non-linearity is likely to depend on the degree of large scale spatial heterogeneity of soil properties and soil moisture conditions. In relatively uniform catchments where it can easily happen that a large portion of the catchment reaches a critical soil water state, catchment response is likely to be similar to that at small scales with threshold processes switching between the two regimes and little hope to capture catchment dynamics from point measurements. In relatively heterogeneous catchments the changeover between regimes on individual slopes is likely to average out, and hence the integral catchment response will be more linear and more predictable from point measurements. This is counterintuitive as more uniform catchments are usually considered to lend themselves more easily to hydrologic modeling.

The study also sheds light on the reproducibility of hydrologic measurements in general. One would generally hope that a number of measurements of the same system at the same time would constrain the system state enough to give similar results when used for hydrologic modeling. This study suggests that this may or may not be the case depending on whether the system is in a stable or unstable range. This results from the non-linear dynamics which can lead to an amplification of uncertainties in the experimental conditions if the system is close to the transition between the regimes. Process models of catchment response often fail to predict the results of detailed experiments if no calibration is allowed. This is usually attributed to incomplete process descriptions and insufficient data. We suggest that another likely reason is the potential non-linearity of hydrologic systems. It may well be that we expect model predictions to be more accurate than is possible due to inherent non-linearities which may amplify data uncertainties.

The influence of the spatial variability of soil moisture and precipitation at different scales on runoff production and infiltration

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modeling catchment response to rainfall events is complicated by the high non-linearity of the processes related to infiltration and surface runoff generation. Therefore, the variability of the governing input data and system parameters cannot be neglected. However, variability on different spatial and temporal scales has different influences on catchment scale generation of runoff. The purpose of this study is to investigate the role of spatial variability of initial soil moisture content as a measure of the hydrological state of the soils and the spatial-temporal variability of rainfall as governing input on infiltration and runoff production in a small catchment. To quantify these effects catchment water and runoff dynamics is simulated, based on comprehensive measurements performed in the 6.3 km^2 large Weiherbach catchment, using the physically based, distributed model CATFLOW [187].

As a first step the spatial distribution of soil moisture is interpolated from 61 point observations using different geostatistical methods such as Ordinary Kriging (OK), Bayes-Markov-Updating (BMU) and Simple-Updating (SU). The latter two procedures allow the use of easily measurable proxy variables as prior information, which can be used for interpolating initial soil moisture patterns. The crucial thing is to choose the right proxy data [18]. In the present study we compare a combination of field capacity and plant water utilisation coefficients, representing the time invariant influence of the distribution of soil types as well as the time dependent influences due to water losses by plant transpiration, to the well known topographical index. BMU and SU with these prior variables give estimated average initial soil moisture values, which are dependent on the given land use and soil type or the topographical index. The feasibility of the used proxy data and interpolation methods is checked by comparing observed and simulated runoff events, based on the OK, BMU and SU estimated initial soil moisture patterns. The "optimum" combination of proxy data and interpolation method is the one that will lead to the smallest bias.

For a further improvement of the modeling results we superimpose additional variability on the initial soil moisture pattern, generated with the optimum combination of proxy data and interpolation method, by means of zero mean geostatistical conditional simulations of the soil moisture, using nested variograms with different ranges and sills. Here the effect of the variability at different scales is investigated and compared. This is done by conditioning several simulations of rainfall-runoff events with CATFLOW on initial soil moisture patterns, which are generated by geostatistical simulation using different ranges to represent soil moisture variability on different spatial scales, and comparing the bias

and the uncertainty of the simulated and observed runoff. In addition the simulated soil moisture patterns at the end of the rainfall-runoff events are compared to interpolated soil moisture patterns on the hillslope and the catchment scale. Possible procedures to replace large number of Monte-Carlo simulations with limited number of well chosen realisations (patterns) similar to the Rosenbluth method [140] are discussed.

Especially when there is a spatial "key structure" as it is the case for the Weiherbach catchment we expect the small scale variability of initial soil moisture, corresponding to short variogram ranges, to be of minor importance for runoff generation on the hillslope or catchment scale. Due to the high erodibility of loess strata the average hillslope in the Weiherbach catchment has a typical erosion catena, with Calcaric Regosols (FAO/UNESCO, 1988; Pararendzina) or Luvisols (FAO/UNESCO, 1988; Parabraunerde) in the top or the mid-slope sectors and Colluvisols at the hill foot (FAO/UNESCO, 1988; Kolluvium). Zehe & Flühler [187] showed in an analysis of 10 plot scale tracer experiments, that the spatial pattern of the macro-porousity on the hillslope scale, which is the most important factor pre-disposing a site for preferential or matrix flow, is strongly influenced by this typical hillslope soil catena. Thus, if this typical spatial soil pattern on the hillslope scale indeed dominates the variability of infiltration and runoff generation, the remaining residues between simulated and observed runoff will be clearly reduced, if additional variability of a range corresponding to the typical range of a hillslope soil catena is superimposed on the optimal interpolated soil moisture patterns.

In the second part of the study the role of the spatial and temporal variability of precipitation is investigated. Rainfall fields are interpolated in space and time at different spatial and temporal scales based on observations at 7 rain gauges. Three dimensional turning band simulation is used to generate conditional space-time rainfall fields. The cross correlation of the different precipitation gauges' time series gives information of the spatial structure. The temporal structure can be inferred from the time series' autocorrelation functions. Nested variograms with different sills and ranges are used for the geostatistical simulation of the rainfall fields. The effect on the runoff production and the infiltration is investigated as a function of the variance and the corresponding range, performing simulations of rainfall-runoff events with CATFLOW with the different rainfall fields. As in the case of the soil moisture we expect again that the influence on the bias of the simulated discharge decreases with decreasing range of the variogram. The resulting soil moisture maps are evaluated at different spatial scales.

The overall comparison of the results corresponding to the different simulated and interpolated initial soil moisture fields on one hand and rainfall fields on the other hand will show to what extent interpolation using external proxy information and conditional geostatistical simulation can contribute to a better modeling of catchment response to rainfall events, but also to a better modeling of catchment scale soil moisture dynamics.

Numerical dissipation and parameter values in the distributed hydrological modeling

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The dissipation of the numerical schemes used to solve the partial differential equations governing groundwater and surface flow has to be considered for the calibration of distributed catchment models. The effects of the numerical dissipation of the finite difference schemes adopted are investigated in this work in order to define the meaning of the model parameters. To this regard, a finite difference distributed model for the continuous simulation of the coupled groundwater-channel flow has been employed using a ten-year hydrological data sequence from a 123 km^2 vegetated steep basin ([119]).Finite difference schemes have been used in order to solve mass and momentum balance equations of the two-dimensional (2-D) saturated subsurface flow and the one-dimensional (1-D) kinematic surface flow. The groundwater flow equations are solved with a one-step explicit 2-D finite difference scheme ([1]), based on the same spatial square grid as the digital elevation model (DEM). The surface flow routing equations are solved with the weighted four-point implicit 1-D finite difference scheme ([60]), based on the spatial structure of the channel network extracted from the grid DEM.Taking into account inadequate knowledge of the small-scale variabilities of soil properties and precipitation data, the model has been developed maintaining the basic components of the hydrological processes represented and minimizing the number of parameters ([69]). The geomorphologic and climatic input data, used by the model in distributed form, are the soil thickness, the DEM, the 15-min rainfall and the monthly temperature. The roughness coefficient is the sole calibration parameter for the surface flow, soil storage capacities and hydraulic conductivity are the parameters for the groundwater flow, the vegetation interception and an evapotranspiration coefficient are the parameters for the hydrological cycle balance. In accordance with the conditions which ensure consistency and stability in numerical schemes, a time step equal to 900 s and a space step ranging between 250 and 10 m were used. The first five hydrological years of the available historical series have been used for the calibration of three model parameters: the effective porosity, the surface hydraulic conductivity and the evapotranspiration coefficient. An automatic optimization procedure consisted in maximizing the simulation efficiency, evaluated in terms of daily and hourly discharges. The simulation efficiency has varied from 87% in the first five-year calibration period to 85.8% in the subsequent five-year validation period.

Model resolution effects on numerical solutions were studied in terms of the space-step size, which influences the topographic representation of the simulated field processes and the approximation of the solutions. Several grid discretizations between 250 and 10 m were used since the DEM extraction phase. This analysis proved that the truncation error of the higher order terms in the finite difference approximation of groundwater flow equation, produces a numerical dissipation which can be balanced with a larger hydraulic conductivity as the space-step size grows. The conductivity parameter can then take on

physically meaningful values only if a very small space-step is used. For greater values, the conductivity parameter must therefore be chosen empirically with increasing values as the grid size increases.

The numerical dissipation of the finite difference scheme for the channel flow simulation is also used to represent the attenuation of the flood peak, to compensate for the fact of having ignored the acceleration and diffusive terms in the kinematic wave approximation [12].

This analysis has shown how some distributed model parameters vary and lack physical meaning because of dissipation of the numerical schemes, which considerably increases as the space-grid step increases.

On the dialog between experimentalist and modeller in catchment hydrology: Use of soft data for multi-criteria model calibration

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A major obstacle in moving forward with conceptual modeling approaches is how to obtain data for internal calibration and validation. Currently, the use of this measured data for model calibration is often limited beyond simple streamflow information despite the general acceptance that internal state information is necessary for ensuring model consistency. The usefulness of having various criteria for assessment of model performance is widely accepted but in most cases there is no suitable hard data available.

The dialog between experimentalist and modeler in catchment hydrology has been minimal to date. The experimentalist often has a highly detailed yet highly qualitative understanding of dominant runoff processes-thus we often have much more information content on the catchment than we use for calibration of a model. While modelers often appreciate the need for hard data for the model calibration process, there has been little thought given to how modelers might access this process knowledge. There exists in addition to hard data (streamflow hydrograph, well record) ?soft data? about catchment hydrology. Soft data can be defined as qualitative knowledge from the experimentalist that cannot be used directly as exact numbers for model calibration but that can be made useful through fuzzy measures of model-simulation and parameter-value acceptability. We argue that soft data represents a new dimension to the model calibration process that might (1) enable a dialog between experimentalist and modeler, (2) specify realistic parameter ranges often ignored in today's automatic calibration routines, and most importantly (3) be a formal check on the 'reasonableness' and consistency of internal model structures and simulations. Previously, when calibrating a conceptual rainfall-runoff model manually, some of this qualitative understanding might implicitly influence the calibration. The search for optimal parameters is thus restricted to certain parameter values and the modeler might visually inspect simulated internal variables such as groundwater levels and consider how reasonable these simulations are. The explicit use of soft data has two advantages: the goodness-of-fit criteria are, while still being subjective, stated a priori and the method can be used in automatic calibration routines. In other words, the procedure injects some experimentalist common sense into the automatic calibration process.

We present a methodology to make soft data useful through fuzzy measures of model-simulation and parameter-value acceptability. The method was first tested with a three-box lumped conceptual model for the Maimai catchment in New Zealand, a particularly well-studied process-hydrological research catchment. The boxes represent the key hydrological reservoirs that are known to have distinct groundwater dynamics, isotopic composition and solute chemistry. The model was calibrated against hard data (runoff and

groundwater-levels) as well as a number of criteria derived from the soft data (e.g. percent new water, reservoir volume etc).

We achieved very good fits for the three-box model when optimizing the parameter values with only runoff (R_{eff}=0.92). However, parameter sets obtained in this way, showed in general a poor goodness-of-fit for other criteria such as the simulated new-water contributions to peak runoff. Including soft-data criteria in the model calibration process lead to lower $R_{eff} - values$ (around 0.86 when including all criteria) but led to better overall performance, as interpreted by the experimentalist's view of catchment runoff dynamics. The goodness of new water ratio evaluated by soft data, for instance, increased significantly and parameter uncertainty was reduced by 60% on average with the introduction of soft data multi-criteria calibration.

A similar model approach was used for other small experimental catchments, located in Sweden and in the USA. The available soft data varied depending on geographical conditions and experimental design. The usefulness of including soft data was tested and the value of these data was compared for the different catchments.

We argue that accepting lower model efficiencies for runoff is worth it if one can develop a more 'real' model of catchment behavior. The use of soft data is an approach to formalize the dialogue between experimentalist and modeler. This contributes to ensure a better process representation of catchment hydrology in conceptual runoff modeling and forces the model to be, instead of being 'right for the wrong reasons', 'less right, for the right reasons'.

Active microwave remote sensing of soil moisture over Europe

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A Physically based algorithm for retrieving soil moisture variable and land surface vegetation cover fraction from the database of Global C-band Radarbackscatter is proposed in this paper. The backscattering contributions from bare soil, vegetation layer, soil beneath the vegetation and soil-vegetation interaction have been taken into account in this method. A technique for solving the nonlinear equations is involved in the retrieval process. Site specific time series and regional distribution of soil moisture, vegetation cover fraction and soil surface roughness are estimated by the developed method over the European continent. Generally the regional distribution of the soil moisture variable, vegetation cover fraction and roughness variable are reasonable. The time series of soil moisture variable has been compared with the local monthly rainfall to validate the developed algorithm, the retrieved soil moisture corresponds with the local monthly rainfall. It is concluded from the calculation and comparison that the determination of soil moisture is feasible from this larger space resolution ERS-Windscatermeter data.

The new integrated hydrological model MOHISE: construction, implementation and results

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The development of an integrated hydrological model is presented. This model, named MOHISE, which stands for 'Modèle Hydrologique Intégré pour la Simulation du cycle de l'Eau' (Integrated hydrological model for the simulation of the water cycle), is a part of the project 'Integrated modeling of the Hydrological Cycle in the Scope of Climatic Changes' supported by Prime Minister's Office – Federal Office for Scientific, Technical and Cultural Affairs of Belgium, in the scope of the general program 'Global Change Sustainable Development'.

General structure of MOHISE MOHISE is a deterministic, spatially distributed, physically-based model, composed of three interacting sub-models: a soil model, a groundwater model and a surface water model, which are linked dynamically and operated in a global structure. The construction of the global structure of the integrated model required the adaptation of the different sub-models in order to run together and the construction of a meta-structure which controls all the integrated model running operations. The meta-structure (Master code) has to synchronise the run of the different models on a multi-node parallel computer and to organise the message exchanges between the different sub-models, as the simulations are performed. This approach leads to several advantages. First, it allows to change any of the sub-model as other numerical or conceptual requirements are needed (e.g. the groundwater sub-models MODFLOW or SUFT3D can be used in substitution of each other). Second, it allows a very flexible general structure, with minimal changes required for the sub-models to be run under the integrated environment. At least, they have to be adapted in order to be able to send and receive messages to the Master code (e.g : water fluxes at different time steps). Third, the water fluxes, at different points in the system, are logged in files for verification and analyses in subsequent post-processing operations.

Coupling principles between the different sub-models The three sub-models are dealing with different compartments of the water cycle. The EPIC-GRID soil model [146] computes a general water budget at the soil surface and in the unsaturated zone, differentiating water between evapotranspiration, overland flow, slow and fast runoff subsurface flows and percolation ; the unsaturated zone includes root zone in relation with crops growth. The surface water model deals with water flows in the river network and the

groundwater model deals with the groundwater flows (so with the base-flow at the discharge points). Water fluxes are exchanged between the three sub-models, at different space locations and over time. To handle these exchanges efficiently, some spatial and temporal mapping procedures have to be developed. These procedures are summarised here.

Surface water distribution The relation between the basin grid cells and the river network is established through 4 different 'parameters' :

- the connectivity matrix : each basin grid cell can be linked to a digitised point in the river network (method of steepest descent on the DTM);
- the distance between the grid cell and the corresponding digitised point in the river network;
- the difference of altitude and the variation of the altitude along each trajectory;
- the delimitation of the watershed located 'upstream' each basin grid cell (and calculation of a "flow accumulation index" for each grid cell).

Starting from the generated connectivity matrixes, the Master code computes the transfer functions from the soil cells (soil sub-model EPIC-GRID) to the river network digitised points (surface water sub-model). These fluxes are logged in files for control and analysis purposes.

Surface water – groundwater exchanges Interactions between rivers and aquifers [36] are expressed as computed water flow rate depending on the difference existing between the piezometric head in the aquifer and the water level in the river, dynamic Fourier boundary condition [27]. The interface between the groundwater sub-models and river sub-model is developed taking into account the fact that it has to be compatible with both codes SUFT3D and MODFLOW. The difficulty to obtain this compatibility is related to the use of different numerical methods (finite element in SUFT3D and finite difference in MODFLOW). In the SUFT3D code, the streams are explicitly discretized by a series of nodes where the exchanged water flow rate is computed [27]. In the MODFLOW code, the discretization with rectangular cells does not allow to keep accurately the course of the river and one cell can be crossed by several rivers. A pre-processing command in GMS allows to automatically assign the river boundary condition to the appropriate cells from the digitised river network.

Soil water – groundwater exchanges The interface between the EPIC-GRID soil sub-model and the groundwater sub-model has been designed taking into account the two possible choices for the groundwater sub-model. The first step consists in distributing in the horizontal plane the percolation flows computed by the soil sub-model. As the horizontal spatial discretization of the groundwater sub-model is not generally identical to the regular grid of the soil sub-model, a spatial distribution algorithm of the results has

to be designed. In a first time, the simplest algorithm has been implemented: search for the location of the centre of gravity of the upper elements (for the finite element mesh) or of the upper cells (for finite difference grid) and attribution of the recharge computed in the cell of the soil model where this point is located. If some elements (or cells) of the groundwater mesh (or grid) are not covered by the soil grid (for example on boundaries), the recharge computed in the nearest cell is used.

If the discretization of the used groundwater sub-model is grid based (like in MODFLOW), a matrix of connectivity can be simply and straightforwardly deduced. If an unstructured finite element mesh is use (like in SUFT3D), a correspondence table between the mesh element numbers and the associated cell of the soil grid has to be built.

To ensure mass conservation in the water exchanges from a sub-model to another, the grid of the groundwater sub-model is chosen as a subdivision of the grid of the soil sub-model. In the case of a connection with an irregular mesh, the exact transfer cannot be done. Tests were carried out to verify if the algorithm of distribution generates acceptable "errors" (i.e. that the eventual error stays in the range of uncertainty of the global water balance). An irregular 2D mesh (with element sizes varying from 100 m to 800 m) has been built using the conceptual model developed in GMS for the MODFLOW code. Tests were carried out with different spatial distributions of the recharge on the regular soil grid (size of the cells equal to 1 km). The maximal difference between the global flow rate given by the soil model and the global flow rate received by the groundwater model does not exceed 0.16 %. That is obviously an acceptable difference with regards to the uncertainty on the actual transfer. Consequently the chosen algorithm seems convenient but final verifications will be carried out for each application with the SUFT3D sub-model. The second step consists in adapting the way of transferring the recharge at the adequate depth. Two ways are used according to the used groundwater program:

- with the SUFT3D sub-model, able to model the flow in the unsaturated zone, the recharge is transferred from the EPIC-GRID soil model at a fixed depth corresponding to the top of the groundwater model; and
- with the MODFLOW sub-model, not able to model the flow in the unsaturated zone, the transfer is entirely computed by the soil model up to the water table. As the water table fluctuates, the recharge is computed for different depths and the used value is deduced from these results according to the depth of the water table.

Integrated model application : Water catchment modeling and Global Change
The MOHISE model has been used in its integrated version to simulate the Gette basin and the Geer basin. Main results will be illustrated and commented. Conclusions and perspectives can be drawn in showing that this integrated tool can be used to assess the effects of climatic changes on the hydrologic and water resources systems at the basin scale.

Statistical Inference for the Location of Catchment Average Soil Moisture Monitoring (CASMM) Sites

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In a statistical/inferential context, information is the sole key to the understanding of complex natural phenomena like the temporal and spatial variation of catchment soil moisture. The recognition of information shortage as a fundamental constraint in catchment hydrology, with accompanying re-prioritisation of financial resources towards increased efforts of hydrological monitoring, should therefore be considered as a milestone breakthrough. As a result, databases with high enough temporal and spatial resolution to reflect generic hydrological catchment characteristics are beginning to emerge. In the work presented here, observations made in six such Australian, New Zealand, and North American catchments are used to infer the statistical characteristics of the generic population of catchment soil moisture. When compared with the characteristics of individual observation sites, the probability of the observation site to reflect generic catchment characteristics is estimated. With high enough probability, the observation site may be considered as a CASMM-site, thus capturing generic catchment characteristics and being well suited to represent the catchment in a monitoring effort. With CASMM-probabilities varying from one site to another, the variation of estimates is well suited for post-hoc analyses of landscape factors influencing the CASMM suitability. The project aims to establish such relationships in models for prediction of the optimal location of monitoring sites in hydrologically unknown catchments. In order to create a statistically robust measure of CASMM probability, several obstacles will be dealt with. Firstly, soil moisture is observed in a temporal scenario characterised by annual variation in patterns of precipitation, temperature, and windspeed. In other words, individual observations are likely to be temporally auto-correlated with non-stationary mean- as well as variance components. The non-stationary mean is primarily represented by inter-seasonal variation on the annual scale, whereas he non-stationary variance component is primarily represented by storm-weather passages within seasons. Since, in the catchments analysed, these atmospherically related processes are densely monitored, they can neither be considered as random, nor as representing the landscape-associated processes addressed with the CASMM probability. To balance their effect, the observed time-series will be filtered with transfer function ARIMA models, cross-correlated to the series of observed external processes which will leave the observed residual variance within individual series of soil moisture to be considered as mainly representing

landscape associated processes, and as being independently random with stationary mean and variance. When the residual series of ARIMA-filtered observations are distributed in the landscape, individual observation sites are overlaid on a topography that, on the catchment scale, governs preferential flow-paths. This means that the wetness of downstream points is partly determined by upstream wetness and that, therefore, covariance is topographically induced within groups of observation sites. To minimise such statistical inter-site dependency, the observed spatial covariance structures will be considered as anisotropic autocorrelation, and balanced with Kriging models. As a result, the residual matrix should reflect the random inter-site variation mainly associated with local characteristics, such as geomorphologic and soil/regolith properties, of individual observation sites. With the resulting residual matrix mainly representing the landscape contribution to the observed inter-site variation of soil moisture, the probability of individual sites representing the generic catchment characteristics can be assessed. There is, however, another obstacle to address before the final analysis, namely the possibility of multiple regional characteristics within individual catchments. In an inferential context, this is synonymous with identifying groups of observation sites with intra-group covariance significantly exceeding the covariance between groups. In the residual matrix of random observations, such multivariate identification is classically accomplished with methods of factor analysis. As a result, the hypothesis to address in heterogeneous catchments will be the existence of CASMM-sites within homogenous regions of soil moisture. To finally design a proper test of hypotheses regarding the existence of CASMM-sites, the meaning of the word homogeneity needs closer examination. It expresses the combined effect of generic mean and variance, and could very well also include higher statistical moments. In other words, individual observation sites should be compared to the generic population with respect to combined location and shape of soil moisture probability density functions. Another important criteria in the design of a proper statistical test, is the relatively small number of observation sites expected within individual homogenous regions. The combined criteria therefore disfavours parametric test methods, in favour of non-parametric methods utilising sums of ranks. Since, furthermore, the individual observation site is an integral part of the catchment with which it is compared, the test variables may be considered as being pair-wise dependent. This reduces the number of possible designs down to a! few non-parametric methods to test the null-hypothesis H0: the probability distribution within a single observation site is identical with the average distribution of the homogenous region. When repeated for all sites within the region, their respective probabilities P(H0) are well suited for the ranking of individual sites with respect to their ability to capture the average probability characteristics of the homogenous region. With a test criteria of P(H0) = a, sites exceeding the criteria may be considered as CASMM-sites, whereas P(H0) measures the probability for individual sites to pass the test. With many sites observed in a wide range of landscape characteristics, the variation of CASMM-probabilities is well suited for post-hoc analysis. As a bonus, the coefficients of best fitted ARIMA and Kriging models are designed for convenient statistical inference on the generic properties of atmospherically and topographically related processes as discussed above.

Spatial Organization of Land-Atmosphere Interaction

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The exchange of water, heat, and trace gases between the land and the atmosphere drives the dynamics of weather, climate, and the hydrologic cycle. Predictive models (from flood forecasting to climate evolution) must capture the spatial and temporal variability of the land surface exchange rates. Progress in this area has been impeded by the computational intractability of the combined dimensionality of the land surface heterogeneity and the physical and biological processes affecting the exchange. Furthermore, efforts to assimilate remotely sensed data into large-scale models must include some basis for dealing with variability in the data at sub-model-scales. In this talk we will examine whether such a high-dimensional problem produces spatial organization that supports the use of low-dimensional models integrating surface properties and exchange processes. We will review results from a combination of field experimentation and computational fluid dynamics tools applied at three ranges of spatial scales: regional (>100 km), landscape (100 m to 10 km), and local (1 m to 500 m). At the regional scale we investigate the organization of biosphere function (with respect to water use) along a climate gradient on the Kalahari Transect (KT) in Southern Africa as observed in a recent intensive field campaign. Analysis of water, energy, and carbon flux data collected along this gradient with a portable tower demonstrates how the high frequency functional control on water and carbon cycling has adjusted to the large scale features of the long-term climate gradient. At the landscape scale we use a Large Eddy Simulation (LES) model of Atmospheric Boundary Layer (ABL) development with remotely sensed land surface (boundary) conditions to explore scale preferences in the feedbacks between surface properties and atmospheric processes. The LES is integrated with boundary conditions from day 221 of the Monsoon90 experiment and analysis is conducted to quantify the transmission of surface heterogeneity information into the ABL. The LES model incorporates: radiant energy availability; spatial fields of remotely observed surface cover, temperature, and moisture; and, the ability to account for the separate contributions of soil and vegetation (i.e. two sources) to the mass and energy exchanges. Analysis of the results reveals that the time-averaged, near surface air temperature field contains spatial variability induced preferentially from variations in surface temperature occurring at scales greater than 500-1000 m. At the local scale we use a higher resolution Large Eddy Simulation model to explore scale organization in the coherent vortices generated at the vegetation-atmosphere interface and transporting mass and energy into the atmosphere. Kelvin-Helmholtz type instabilities are found to be generated at the peak velocity gradient location just above the canopy (analogous to a mixing layer). These coherent structures have characteristic length scales that

depend on the canopy morphology. Through the LES we characterize the evolution and impact of these structures on canopy-atmosphere exchange of mass and energy. We also extract a one-dimensional projection of these structures that guides the observations of these flux events in high frequency time series collected from towers in the field.The three scale brackets considered in this talk combine to represent much of the spectrum of land surface variability. The self-organization highlighted in this talk motivates future work toward developing a more tractable low-dimensional view of the essential land-atmosphere dynamics.

4 Model calibration
Chairman: S. M. Hassanizadeh

Assimilation of data for the construction and calibration of watershed

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This talk will discuss some issues related to the task of building a useful catchment-scale hydrological model. Clearly, the model should be capable of accurately simulating the watershed behaviors that are of interest. However, we are also interested in it being able to provide insight into the potential behavior of the catchment under changes in hydro-meteorological conditions (e.g., precipitation, temperature) or catchment structure (e.g. land use). A major concern in building such models is that of appropriate (necessary and sufficient) model complexity. The talk will report on recent research in which multi-criteria methods, that allow combining of the strengths of both manual and automatic calibration approaches, are being used to guide the process of model development and to identify which aspects of process heterogeneity require explicit representation.

A dynamic identifiability approach to the evaluation of conceptual hydrological models

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Many, if not most, hydrological model structures currently used can be classified as conceptual. By this we mean that the structure is specified *a priori*, and (at least some of) the model parameters do not have a direct physical interpretation, in the sense of being independently measurable, and have to be estimated through calibration against observed data. The modellers task is the identification of an appropriate conceptual model structure and a suitable parameter set for a specific case, *i.e.* a given modeling objective, catchment characteristics and data set. Experience however shows that this can be very difficult. Various parameter sets, often widely distributed within the feasible parameter space and sometimes even different conceptualisations of the hydrological system can yield equally good results in terms of a predefined objective function. The problem is increased by indications that, due to structural inadequacies, a single parameter set! might not be enough to describe all response modes of a hydrological system. This ambiguity has serious impacts on parameter and predictive uncertainty, and therefore limits the applicability of conceptual models, e.g. for the simulation of land-use or climate-change scenarios, or for regionalisation studies.

One reaction to this problem of ambiguity of system description is the search for calibration methods with higher *discriminative power*. This potential method should make better use of the information contained in the available time-series and also indicate structural inadequacies to provide an objective analysis of the suitability of a model and model structure respectively.

A new methodology for the identification and analysis of conceptual hydrological models called *DYNamic Identifiability Analysis* (DYNIA) will be presented [174]. This builds on a toolbox developed at Imperial College for Monte-Carlo analysis of model structures and parameter identifiability using techniques based on regional sensitivity analysis [149]. The new approach is based on the evaluation of the model performance as a function of time and therefore makes it possible to use more of the available information in a calibration procedure. By reducing the loss of information through the aggregation of residuals in time, DYNIA can give insight into the model behaviour during different response modes and highlight structural inconsistencies. It can also be used to segment the hydrograph to define different objective functions thus maximising the information retrieved from a time-series. An example will be shown based on rainfall-runoff modeling! of a UK catchment where DYNIA is applied to a relatively simple model structure containing typical conceptual elements.

Identification of distributed parameters in hydrologic models

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Introduction Complex distributed models loose much of their strength and advantages to lumped models when their distributed parameters can not be identified. This is however a general problem in distributed models, as their parameters typically produce good simulations over almost the entire range of any single parameter [148]. In this context Beven [13] stated that the principle of parsimony does not appear to be widely articulated, possibly because reductionism coupled with a deep belief in the correctness of scaling up small-scale physically based models has been the dominant paradigm.

On the other hand, parsimonious models are usually limited to simulating the response to which they have been calibrated under catchment conditions (climate and land use) which are similar to those encountered in the calibration [96]. Thus, a simple model cannot be relied upon to make meaningful extrapolative predictions. A complex model may have the potential but, because of information constraints, may be unable to realise it [96].

A good calibration requires a data set that is able to identify the parameters, although problems in calibration and identification will not necessarily disappear with the availability of more and better field measurements [70]. They state that the informativeness of the data is far more important than the amount used for model calibration. This is the case when the observations yield a summation of many elements that should be identified separately as for instance base flow and runoff components. The same happens to an area with mixed composition that is drained to a single observation point, while each hydrologic element responds differently. As only the result of the sum of all these elements is known, is it then in general not possible to identify the typical parameters of the different elements. Also the structure of the model itself can cause problems in the identification process, when the parameters are correlated to each other or non sensitive.

A simultaneous use of more than one signal can however improve parameter identifiability [37]. Mroczkowski et al. [117] concluded out of their study that when only streamflow data are available for calibration and validation, only weak statements about model structure can be made. At the other hand, it is important to keep in mind that augmenting stream flow with other response time series does not necessarily reduce the model uncertainty and improve the identifiability of model [96].

This study aims to improve the parameters identifiability of a semi-distributed model by multi-point calibration. The analysis is based on the comparison of the identifiability of the parameters after single point and multi-point calibrations.

Multi-objective calibration Several methods can be used to aggregate individual objective functions to a single objective criterion [113]. This global criterion, representing the errors, is then minimised and its minimum corresponds to the optimal parameter set.

Important here is the weight of the individual objective functions in the global criterion. When the weight of an objective function is too low, it will just be ignored in the search procedure. The problem is that the absolute value of the interaction between the objective functions is not known. Due to this, a simple 2 criteria case can require several different weighting schemes for a better optimisation [37, 113]. Apart from this mathematical problem, there are also some subjectivities that play a role. The modeller could have a preference for a certain objective function, while others can be of minor interest. According to Gupta et al. [70] the derivation of a multi-objective problem to a single-objective problem must necessarily involve some degree of subjectivity.

The aim of calibration in calibration problems is to minimise the error between the measured and the calculated model output, what is mathematically translated to an objective function. In a multi-point calibration, this has to be done for several outputs simultaneously. The corresponding objective functions should thus take equal part in the calibration process. This is achieved in a new methodology whereby several objective functions are reduced to a single global optimisation criterion excluding the weighting problem. This methodology is based on the normal distributions of errors. It operates in several steps. For each objective is first the mean and variance of their objective functions calculated, based on runs where the parameters are sampled randomly. The mean and variance are in the further steps used to calculate the cumulative frequency function for each objective function, which is in the range 0-1. The sum of these frequency functions gives finally the global optimisation criterion for each model run. This global optimisation criterion will be minimized by the SCE-UA method [44].

Shuffled complex evolution method (SCE-UA) The effectiveness of the calibration depends highly on the search algorithm [75]. The SCE-UA shuffled complex evolution method combines several search methods and can shortly be described as an approach that treats the global search as a process of natural evolution [44]. As it search over the whole parameter space, it finds the global optimum with a success rate of 100.

Measure of identifiability of parameters Non-sensitive parameters can be detected by a sensitivity analysis. The overall identifiability of the parameters can be derived from the Fisher Information Matrix or FIM [177], which is the inverse of the parameter covariance matrix obtained from the global criterion near the optimum [59].

The hydrologic simulator ESWAT ESWAT has been developed by the authors with the aim of integrating the water quality and quantity processes at river basin scale [165]. The original SWAT model [4] is hereto extended by including a new infiltration module, a convolution module for the runoff components, a new river routing module and a river water quality module. In addition, the calculation time step has been reduced from daily to hourly or less. Infiltration and erosion processes operate on a user defined time step - a fraction of an hour - to get a better description of these processes.

Case study Calibrations are performed in the Dender basin (Belgium). The river Dender is a tributary of the river Scheldt and drains an area of 1384 km^2. The river reacts quickly to precipitation events. After storms, the flow can rise to over 100 $m^2\,s^{-1}$, while during

the summer the flows are less than 1 $m\,s^{-1}$m/s. These irregularities are tempered by a number of sluices built on the main channel to guarantee ship-traffic. The main channel is also partly canalised.

Single point calibrations are performed for the flows of 3 tributaries and 1 for the main channel outlet using each time about 13 parameters. The multi-point calibration includes a simultaneous calibration on the flows of 3 tributaries and one point on the main channel, to define the land use, soil and other geographically distributed parameters.

The flows of the tributaries are calibrated simultaneously by aggregating their objective functions. The same parameters as in the single point calibration were used, however sharing the soil type, the land use type parameters and the routing parameter. This gives 8 shared and 6 individual parameters, making 32 in total.

Step-wise physically-based construction and calibration of a lumped conceptual rainfall-runoff model, based on the model uncertainty-structure

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With a lumped conceptual modeling system, runoff of rain water from a hydrographic catchment can be described in a spatially-averaged way. The system lumps, in a broad sense, the highly complex soil processes and properties into a few processes and parameter values. Many such modeling systems have been developed. A few examples are mentioned here: the Dawdy-O'Donnel modeling system [Clarke, 1994], the UK Institute of Hydrology Lumped modeling system [31], the NAM modeling system of the Danish Hydraulic Institute [41], the Stanford Watershed Model [35], the Sacramento modeling system of the US National Weather Service [23]. Most of these systems have a similar model structure. In this structure, storage elements are used to model the storage of water at the surface (interception storage), the unsaturated zone (root zone and lower zone soil moisture storages) and the groundwater. Reservoir models moreover describe the routing of the three runoff subflows: surface runoff, interflow (runoff from the vadose zone) and groundwater flow (baseflow). In spite of this general structure, the detailed structure and complexity of the modeling systems can be very different. The subflow-separation processes (infiltration processes) can be modelled by linear or more complex relations. The routing processes can be represented by several types of reservoir models (linear, non-linear, cascade, etc.) or more general unit hydrographs. The implementation of a specific modeling system may be complicated due to assumptions in the model structure which may not be valid. The consideration of only two subflows (quick flow and slow flow) and the consideration of model input and output on a daily basis (together with the corresponding effect on the model structure) are two examples of such assumptions. Whenever a modeling system with these two assumptions is implemented for a watershed for which interflow results and runoff is highly variable on an hourly basis, a poorly identifiable and biased model with large model uncertainty can result. It is the personal experience of the author that this identifiability problem of lumped conceptual rainfall-runoff models occurs often in practice. Whenever automatic or numerical calibration techniques are used instead of trial-and-error, the problem takes even larger proportions through the subjective choice of the objective function , the existence of local minima in the objective function, and experience of the modeller that is not used. Also due to over-parameterization, identifiability problems occur. Beven stated that 3 to 5 parameters should be sufficient to reproduce most of the information in a hydrological record [11]. Jakeman and Hornberger have shown this in a more objective way by applying numerical time series techniques [81]. They concluded: for catchments in temperate climates but over a tremendously wide range of scales, only a handful of parameters can be reliably estimated from rainfall-runoff data . However, by considering inductive information (prior information, e.g. experience), the author believes that this number can be increased. Many authors have already addressed the previously mentioned

complications of implementation of conceptual rainfall-runoff modeling systems. Solutions have been presented both in terms of calibration technique and model structure. Among the calibration techniques, Duan et al. have developed advanced optimisation techniques [130]. These continue to have the large disadvantages of numerical calibration methods: no use of prior information and a less-transparent calibration. The data-based modeling methodology of [82, 176, 186, 98] solves the identifiability problems of conceptual rainfall-runoff models. Two examples of the corresponding modeling systems are IHACRES [103] and HYCOM [98]. They use a very simple mechanistic model structure, mostly of the hybrid type as it combines a simple conceptual or empirical non-linear rainfall loss model with a generalized linear storage model. The structure of the linear storage model is identified and the parameters calibrated in a data-based way using time series analysis techniques. As a disadvantage, these modeling techniques do not make use of inductive information and, as a result, the derived model structure may be too simplified. The modeling techniques are based on the uncertainty structure of the model, but in a simplified way. Many assumptions are made about this structure that may not be valid: independency and stability of the uncertainties in the model results. The different uncertainty sources are not considered separately and the calibration is not transparent. In the study presented, a modeling procedure is presented that solves the problems mentioned. To meet the complication of inadequacies in an assumed model structure, the modeling methodology starts from a general model structure with similar elements as those of existing modeling systems, but with no detailed description of the subflow separation and routing processes. The model structure is not considered fixed, but sought in a case-specific optimal way. In this way, the construction of the detailed model structure can be considered as part of the calibration procedure. The detailed model structure thus depends on case-specific conditions such as slope, area, soil type, land use, groundwater depth, etc. of the catchment. This is different from most existing modeling systems in which the detailed model structure is more or less fixed and only the model parameters are case-specific. By calibrating the parameters of the different sub-models (routing models, soil moisture storage model, subflow-separation processes) as independently as possible, the calibration becomes transparent. In the procedure, reverse river modeling and a subflow separation procedure is applied based on recursive digital filters. One parameter of the filters is time variable and is a direct measure of the rainfall fraction that contributes to a certain subflow. By re-calibrating this parameter in time, the time variability of the subflow-separation processes is extracted from the data. This is additional information derived only from the river discharge time series by maximizing the use of the physical knowledge about the main processes involved in the system. Model structure refinement and calibration can be based on this additional information, leading to a well-specified model structure with unbiased model parameters. As a result of the transparency of the model calibration, also a transparent uncertainty structure is derived for the model. This uncertainty structure includes model-structure uncertainties for the different sub-models. Based on these uncertainty assessments, model calibration can be performed in a statistically optimal way, eliminating the bias in the model structure and parameters at the same time. In the uncertainty analysis, rainfall input uncertainties are considered first

independently following [179]. The remaining uncertainties, after subtraction of the discharge measurement errors, can then be considered as model-structure uncertainties for the subflow separation processes. As in the deterministic model structure, a lot of assumptions / simplifications have been made in the description of the uncertainty structure of the model. The parameter uncertainties, for instance, were neglected when compared with the input uncertainties and the model-structure uncertainties. This is motivated by the fact that only the most important features of the uncertainty structure have to be described. Indeed, it would not be meaningful to derive an uncertainty structure that is much more detailed than the deterministic conceptual model. A complex probabilistic model has the same problems as an over-parameterized or over-specified deterministic model. It is not useful practically. As with the deterministic model, the probabilistic models and the model uncertainty structures in the present study can be called parsimonious and conceptual.

Multi-Criteria Calibration of Water Quality Models

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Models of stream chemical composition have become valuable policy and research tools, for investigating questions involving atmospheric deposition, climate change, land-use change and land management impacts. However, the inability to develop improved parameter estimation methods for these models has been a constant challenge. If this challenge could be met, it might be possible to use multi-response data to evaluate distributed hydrologic and water quality models. Much work remains on this topic but calibration techniques that use the multiple response nature of stream chemical composition have shown promise, e.g. [37] and [117]. In this paper we seek to investigate the use of multi-criteria techniques based on Pareto rank methods and how they can be used to evaluate and improve the structure of distributed water quality models. Two different case studies will be discussed, both involve the application of the Alpine Hydro-chemical Model (AHM) to the Emerald Lake watershed. The first involves the proper selection of calibration criteria and the second involves using multi-criteria methods to determine the optimal level of spatial complexity that can be incorporated into distributed models of stream chemical composition. We applied a multi-criteria search algorithm to the AHM model of the Emerald Lake watershed, Sequoia National Park, California. There were a total of 21 available chemical and hydrologic criteria for determining model performance. We selected 4 subsets of these criteria to be used in the multi-criteria analysis using three different methods. The first set used the criteria with the least correlated observations for the Emerald Lake watershed. The second set consisted of the criteria with the least correlated RMSE values. Finally, two sets of criteria were chosen using the results of a multi-criteria sensitivity analysis. The results indicate that correlation of stream chemical and discharge observations was a poor method of selecting criteria for multi-criteria analysis. The best method was to use the set of criteria selected via a multi-criteria sensitivity analysis. This method takes into account information about the watershed and the watershed model. The implication is that when using multiple responses to determine the hydrologic or geochemical properties of a watershed it is important to take into account the preconceived notions (models) that exist for the watershed of interest. Also, our results show that multi-criteria parameter calibration methods can improve estimates of hydrologic and biogeochemical processes in a watershed water quality model. The multi-criteria calibration we conducted was also able to identify a flaw in the current representation of mineral weathering within the AHM model of the Emerald Lake watershed. The second case study investigates three different levels of spatial aggregations of the AHM model of the Emerald Lake watershed in order to determine the relative importance of a more versus a less spatially aggregated model. We expect that the simplest model (lumped or 1 unit of aggregation) will lead to a high degree of precision in parameter estimates but not provide an accurate assessment of

the processes occurring in the watershed. The most spatially complex model (5 different aggregation units) will result in imprecise parameter estimates and thus not provide an opportunity to really judge the accuracy of the model in a spatially aggregated state. The middle-ground model (3 different aggregation units) is expected to give a relatively precise estimate of parameters but also manage to stand up to evaluation tests better and thus will be considered the best level of spatial aggregation.

These results are preliminary in nature and only begin to show the possible uses of multi-criteria methods to investigate model structure and estimate parameters for distributed water quality models. Much work remains to be done in learning how multi-criteria tools can be applied to multi-species multi-flux models such as the one discussed in this paper.

Multi-scale calibration and validation of a distributed hydrological model on a farmed catchment

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Management of land and water resources of agricultural catchments has emerged as an environmental priority due to the effects of land-use on runoff, erosion and pollutant transport. Compared to natural catchments, hydrological processes in agricultural catchments are influenced by the agricultural land-use, the division of the landscape in fields and the presence of ditch networks, which are significant man-made hydrologic discontinuities in controlling flood generation. In effect, agricultural operations like tillage have an important influence on local surface runoff infiltration by altering soil hydrologic properties. Also, the ditch networks influence water transfer from the fields to the catchment outlet and flow exchange between surface and groundwater since the ditches don't necessarily follow the steepest slope of the catchment surface topography.

To predict the effects of land-use change in agricultural catchments, one needs to use distributed models. Although it was once sufficient to model catchment outflow, it is now necessary to estimate outflow at the field scale, and to characterise surface and groundwater flow. These flow characteristics are the driving mechanisms of sediment and nutrient transport in landscapes and unless they can be predicted reasonably well, water quality models cannot be expected to adequately simulate sediment and nutrient transport. The parameters of distributed models cannot, in general, be obtained directly from measurable quantities of catchment characteristics, and hence model calibration is needed [147]. Model calibration and validation is still a crucial issue in hydrology and is usually limited to comparing simulated and measured outflow at the catchment outlet, while many other flows are also measured at the sub-catchment scale [184, 107]. This is especially true for distributed models, for which multivariable and multi-scale validation procedures are needed. Such an approach has been tested on the Roujan catchment (Southern France) using the distributed model MHYDAS [115] which attempts to take into account the main characteristics of farmed catchments during flood events. The objective of the present study is to formulate and analyse a calibration strategy for MHYDAS at two spatial scales, the whole catchment and the field (corresponding here to a sub-catchment). In the following, we present the main characteristics of the studied catchment and fields, the hydrological model MHYDAS, the parameterisation and calibration procedures, and describe the main results.

The study area is the farmed catchment of Roujan (0.91 km^2) located in Southern France. The catchment is mainly covered by vineyards and is divided into 237 fields. The drainage network is formed by man-made ditches and generally follows agricultural field limits. The basic instrumental design consists of rain gauges, stream flow recorders, piezometers and

tensio-neutronic sites. In an attempt to describe spatial variability of runoff, discharge is measured at three gauging stations at the outlets of the basin (0.91 km^2), a non-tilled field (1200 m^2) and a tilled field (3240 m^2) (to control weeds, tillage is made one to three times each year during the growing period between March and July). The sensors are read every minute. A network of piezometers has also been installed to measure the spatial variation of the water table level on weekly basis. The major runoff events are usually caused by high-intensity short-duration storms, and are well representative of the hydrology in the Mediterranean zone. The analysis of the general characteristics of the runoff events from 1992 to 1999 showed that the runoff coefficient at the field scale varies between 0 and 80%, and at the catchment scale between 0 and 68%. The main hydrological processes are runoff and infiltration at the field scale and the water exchange between the ditch network and the groundwater. The infiltration/runoff process depends on tillage practices; we distinguish two main situations: a) flood events occurring just after the fields of the catchment were tilled and b) flood events occurring a long time after tillage, when soil crusts are present again on the soil surface. The interaction between the ditch network and the groundwater depends on the water table; we distinguish two cases: a) high water table, generally in autumn, winter and spring and b) low water table, generally in summer. To study these different hydrological situations, eighty four flood events measured between 1992 and 1999 were analysed and classified according to the date of tillage and the groundwater level.

The distributed model MHYDAS subdivides the basin into "hydrological units" taking into account the hydrological discontinuities of farmed catchments. In this application, the Roujan catchment was subdivided into hydrological units corresponding either to field parts, or fields subdivided into sub-catchments. Over each hydrological unit, MHYDAS simulates Hortonian mechanisms of surface overland flow. Infiltrated water is assumed to flow vertically through an unsaturated layer from where it can flow to the groundwater. The flow exchange between the ditch network and the groundwater is calculated using a simple Darcian. The unit hydrograph is used to route surface runoff at the scale of each hydrological unit, and the diffusive wave equation is used for flood routing through the ditch network. Evaporation is not represented since the purpose of the model is to simulate individual flood events. MHYDAS requires the knowledge of the spatial distribution of parameters for each hydrological unit. Three kinds of parameters can be distinguished: those extracted from DEMs, those obtained from field observations and those calibrated. Geometrical characteristics, such as the area, the mean slope and the distance to the reach for a given hydrological unit, the length and the mean slope for a given reach, were automatically extracted from a Digital Elevation Model. The parameters measured or observed in the field were geometrical characteristics of the ditch network such as reach depth, reach width, together with soil water properties and aquifer geometry. Soil properties, such as the residual water content and the water content at natural saturation were calculated from field observations and considered as mean values over the whole catchment. The calibrated parameters were the hydraulic conductivities of the hydrological units, the exchange coefficients between the reaches and the groundwater, and the average value of the Manning coefficient for the ditch network.

Flood events between 1992 and 1995 have been used for model calibration and from 1996 to 1999 for model validation. First, the calibration was performed separately for two categories of flood events (high groundwater level and low groundwater level) by iteratively seeking, for each flood event, the values of the parameters that enabled the most accurate simulations of the observed hydrographs at the outlets of the two experimental fields and of the catchment. Of a large number of objective functions that have been defined in the literature [42], the main criterion of MHYDAS performance are predicted to observed total runoff ratio, predicted to observed peak discharge ratio, and the commonly used [118] coefficient. The calibration process was subdivided in two main steps. In the first step, the hydraulic conductivities of the non-tilled and tilled vineyards were calibrated using the hydrographs measured at the outlets of the two experimental fields. In the second step, the spatial distribution of hydraulic conductivity over all the hydrological units, was considered to be known and the other parameters were calibrated using the measured hydrograph at the outlet of the whole catchment. The exchange coefficients between the groundwater and the ditches and the value of the Manning coefficient was calibrated. Using the calibrated parameters, the validation of the model was also made at the scale of the two fields and the whole catchment.

The analysis of results shows that there can be a multitude of parameter combinations that are "equally good" and agree with the concept of "equifinality of parameters sets" introduced by [14]. The value of calibrated parameters depend on the objective function, the quality of data, and the spatial distribution of parameters over the hydrological units. Differences between measured and observed hydrographs are discussed and errors are related to errors in recorded observations and simplifications inherent in the model structure and parameterization. This calibration exercise shows clearly the usefulness of such a multivariable and multi-scale approach to the validation of distributed models. This is necessary, for instance, to further constrain models which have many degrees of freedom, for a more efficient assimilation of remote sensing data in hydrological models, and for better coupling between hydrological and solute transfer models as is needed for land use change studies. Progress in this direction depends directly on the availability, which is still too limited, of good quality, complete, long-term data sets for the variables and parameters involved in the water cycle at the catchment scale.

Deriving catchment-scale water and energy balance parameters using data assimilation based on Kalman Filtering

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Our ability to model regional-scale water-cycle components is hampered by two types of uncertainties. First, we do not have a suitable mathematical representation for the key land surface processes at the catchment scale. Second, for those processes adequately parameterized, we do not know how to aggregate or disaggregate the available information to derive the boundary conditions and the parameters, which are representative of that scale. We have to rely therefore on model approximations of the system's dynamics (and its associated uncertainties), whilst improving our description of the dynamics by incorporating observations (and their related uncertainties). The performance of a model is usually assessed via a calibration-validation methodology, which assumes that the model is "perfect". Discrepancies between simulations and observations are interpreted as the consequence of incorrect values of the model's parameters. The most sensitive parameters are then adjusted to minimize the difference between observations and simulations. In addition, physical realism may also sometimes be used as a surrogate tool to accept or reject the parameter value obtained by the minimization procedure. The parameter set obtained through the minimization over a certain period is then used at any other time, which means that we assume that the minimization period is representative of most hydrological situations. Since we can not adjust the parameters once they are produced by this minimization, we have to rely on assimilation techniques to correct the state variables themselves if a deviation to the observed state appears at any later time. Here, we present a method called "sequential minimization" which combines both Kalman Filter assimilation and a Cost Function minimization. This method produces parameters that are compatible with the way we will use the model later on, that is in an assimilation way. It is used here as a statistically-based scaling tool to derive effective parameter for a 27 km^2 catchment in SE Australia by assimilation in a Soil-Vegetation-Atmosphere Transfer (SVAT) model of sub-catchment scale soil water content observations and land surface temperature measurements obtained over a period of 14 months. Since the Extended Kalman filter's accuracy is limited by the validity of the linearization around the mean state, we compare it with the Ensemble Kalman filter based on Monte-Carlo techniques and the full variance propagation. Derived parameter sets with and without the Extended Kalman Filter (EKF), as well as by hard updating, have been found to be very similar. here we discuss several explanations for this result. First, for most storms and inter-storm periods, vertical soil moisture fluxes occur at a potential (i.e. forced) rate and do not depend on the actual moisture level. This forcing resets the values of soil moisture content and the adjustments by EKF are always of smaller magnitude. Second, soil moisture

content exerts a strong positive feedback on the soil moisture fluxes, and thus a strong negative feedback on the soil moisture level. This implies that biases in the simulated soil moisture content always result in a stronger than true restore term, forcing the soil moisture level towards an equilibrium level. Even if the corrections performed by the EKF method do not affect parameters estimation, they provide us with an indication of the deficiencies in the sampling methodology. Indeed, a lack of measurements for the elevated parts of the catchment is revealed for the last part of the study period when the model can not explain the steady soil moisture levels no matter what parameter values are selected. EKF performs well during that period and can assist in evaluating the subsurface inflow from the upper parts of the catchment as well as assessing its uncertainty. Finally, we have generated a synthetic data set showing which hydrological situations will produce different parameters if the EKF is used or not. We discuss then the relevance of the method for long-term or short term applications.

Assimilating remotely sensed soil moisture and latent heat fluxes in a distributed hydrological model

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In hydrology, models are used to make predictions about hydrological processes in both time and space. A well-known method to check model calculations is to compare the model results with field measurements. In case of big differences, one or more model parameters will have to be adjusted to improve the model calculations. This process is called calibration. Another, rather new, method is data assimilation. Data assimilation is a procedure to provide time-dependent spatially distributed estimates of a dynamic system using observations from various sources and physical constraints in an efficient way [167].

It is the objective of this study to investigate whether remotely sensed soil moisture and latent heat fluxes can be used for data assimilation in order to improve model calculations. In this study the catchment Drentse Aa (300 km2) in the northern part of the Netherlands is chosen as study area. For this area both a distributed hydrological model (SIMGRO) as well as processed remote sensing data (SEBAL) were available. As year of study 1995 is chosen because this was a relatively dry year, in which evapotranspiration reduction occurred.

For this study the following research questions are defined:

1. How do the model calculations compare with the satellite-based calculations concerning evapotranspiration fluxes and soil moisture?

2. Can data assimilation contribute in the process of analysing distributed hydrological models like SIMGRO?

In the Drentse Aa some lateral moraines are situated originating from the glacial periods in the Pleistocene epoch. During the Holocene epoch a natural brook system with deep brook valleys was formed. The Drentse Aa mainly consists of sandy soils. Most part of the area is used as grassland. At the higher parts also forest exists.

The SIMGRO model (SIMulation of GROundwater flow and surface water levels) is a physically based finite element model. The model simulates the flow of water in the saturated zone, the unsaturated zone and the surface water in an integrated manner. The calculation of the evapotranspiration is based on the Makkink equation. Reference evapotranspiration in combination with crop factors results in a potential evaporation per

crop. To calculate the actual evapotranspiration a linear relation between evaporation reduction coefficient and soil moisture is used.

Throughout the area, the discharge peaks are on average simulated too low by the SIMGRO model. The base flow at the outlet point is simulated much too high. It can be concluded that there is too much drainage calculated, also in the summer, in the northern part of the Drentse Aa. In the Drentse Aa model a lot of water flows over the southern boundary into the area and a lot of water flows over the eastern boundary, leaving the area. This is probably not correct and is most likely caused by loss of inhomogeneity in the geo-hydrological schematisation REGIS.

Surface Energy Balance Algorithm for Land (SEBAL) is a relatively new parameterisation of surface heat fluxes based on spectral satellite measurements. SEBAL requires spatially distributed, visible, near-infrared and thermal infrared data. For this study images of the NOAA-AVHRR satellite are used, which have a spatial resolution of one by one kilometer. The satellite passes over twice a day. In 1995 twenty-one satellite images could be used because cloud free days are required. The calculation of the evapotranspiration in SEBAL is based on the Penman-Monteith equation. In case of a satellite image the instantaneous energy balance can be solved, giving together with some assumptions a good estimation of the actual evapotranspiration. In this study, a constant minimal crop resistance is used in the Penman-Monteith equation to derive the potential evaporation. The soil moisture content is estimated in SEBAL by using a non-linear relationship between evaporative fraction and soil moisture content based on field measurements from south Spain and Kansas.

After comparison of the model calculations and remote sensing data a simple 'statistical correction or steady-state filtering' data assimilation scheme based on latent heat fluxes (actual evapotranspiration) is used.

The area averaged actual evapotranspiration calculated by SIMGRO and calculated by SEBAL during the period April-September show a high correlation and their relationship is approximately one to one. The area averaged potential evapotranspiration calculated by SIMGRO and calculated by SEBAL during the period April-September also shows a high correlation but SEBAL systematically calculates higher values than SIMGRO. The area averaged relative soil moisture content calculated by SIMGRO and calculated by SEBAL during the period April-September shows no correlation at all. The values calculated by SIMGRO are systematically higher than the values calculated with SEBAL. Most probably the values calculated by SIMGRO are more reliable than the values calculated by SEBAL. The main reason for this is probably the relationship between evaporative fraction and soil moisture content that is used in SEBAL, which is inappropriate for Dutch conditions.

Data assimilation based on latent heat fluxes results in a spatial distributed actual evaporation that is probably closer to reality. In the assimilated model, the eastern part of the Drentse Aa area has become wetter, resulting in higher yearly actual evapotranspiration compared to the model calculations without data assimilation. As mentioned above the groundwater level is probably calculated too low in the model, due to loss of

inhomogeneity in the geo-hydrological schematisation. In case of deep groundwater levels (beneath approximately one meter) SIMGRO calculates the soil profile too dry. However, the simulated discharges in the area do not improve. This is probably caused by the linear relationship between evaporation reduction and soil moisture content that is used in SIMGRO. Due to this linear relationship it is impossible to increase the soil moisture content of a node more than the soil moisture content corresponding to the reduction point.

Data assimilation as applied in this study promises great potential for analysing distributed hydrological models like SIMGRO.

Automatic calibration of an integrated hydrological catchment model

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Traditionally, calibration of hydrological catchment models has been performed manually using a trail-and-error parameter adjustment procedure. The process of manual calibration, however, may be a very tedious and time consuming task, depending on the number of free model parameters and the degree of parameter interaction. Furthermore, because of the subjectivity involved, it is difficult to explicitly assess the confidence of the model simulations. Due to this, a great deal of research has been directed to development of more effective and efficient automatic calibration procedures.

In recent years, application of automatic calibration routines in hydrological modeling has advanced considerably. Adaptation of such routines, however, has evolved in various directions in different application areas. For parameter estimation in groundwater modeling, gradient-based local search techniques have mainly been applied (e.g. [111]). In lumped, conceptual hydrological models, population-evolution-based global optimisation methods, such as the shuffled complex evolution algorithm [130], have shown to be more efficient. Application of automatic calibration in complex, integrated and distributed hydrological catchment models is an ongoing research area with only very limited experience.

In this paper, automatic calibration of the MIKE SHE integrated hydrological modeling system is considered. Application of automatic calibration routines for this model is a complex problem due to the potential large number of model parameters and the highly non-linear model dynamics. A proper parameterisation of the model and identification of key calibration parameters is extremely important in this case. The proposed calibration scheme considers calibration of the following process descriptions and model parameters:

(1) Groundwater zone component. Hydro-geological parameters for different geological units. (2) Unsaturated zone component. Saturated hydraulic conductivity and empirical conductivity curve parameters for different soil types. (3) Drainage system component. Time constants for routing of water in drainpipes, ditches and canals. (4) River-aquifer interaction component. Leakage coefficients for the riverbed material in different branches.

The calibration problem is formulated in a general multi-objective context in which different objective functions that measure various process descriptions can be optimised simultaneously [70, 107]. In this respect, model calibration can be performed on the basis of multi-variable measurements (i.e. both piezometric head and river runoff measurements), multi-site measurements (i.e. several head and runoff measurement sites distributed within the catchment), and multi-response modes (i.e. objective functions that measure various response modes of the hydrological processes such as e.g. the general water balance, peak flows, and low flows). The shuffled complex evolution algorithm is applied for the optimisation.

A test example is presented that illustrates the use of the automatic calibration scheme and compares with an expert manual calibration. Different sensitivity tests are performed that demonstrate the various trade-offs between the calibration objectives with respect to the use of different calibration data and objective function measures. In addition, the sensitivity with respect to the model parameterisation is outlined. In this regard, a calibration strategy is suggested in which different process descriptions can be calibrated stepwise.

Potential evapotranspiration: its effect on the modeling of the hydrological cycle of a medium-sized catchment with the MIKE SHE code

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Actual evapotranspiration (ET_{act}) plays an important role in the hydrology of a catchment together with other processes such as precipitation, runoff and infiltration. Its proper modeling depends not only on the selection of an appropriate estimation method but also on the availability of realistic estimates of the potential, also called reference, evapotranspiration (ET_p) time series.

In this study, three scenarios considering two variations of the classic Penman equation were inspected for the generation of time series of ET_p. Scenario A included a modified Penman equation using available data of the incoming solar radiation (R_s) and a set of literature-advised coefficients [132]. Scenario B considered the modified Penman equation using available R_s data and a set of coefficients recommended for Belgian conditions [159][132][122]. Finally, the scenario C made use of the FAO Penman-Monteith equation in conjunction with measured R_s data and a set of literature-advised coefficients [3]. For the analysis of the performance of the scenarios, the data from the Belgian stations Bierset, Ernage, Ukkel and St. Hubert were used in the period [01-Jan-1967, 31-Dec-1995]. The available data included information about wind speed measured at 2 m above surface (u_2), mean daily temperature (t_{mean}), actual vapour pressure (e_{act}), relative sunshine duration (n/N) and R_s. The calculated crop potential evapotranspiration (ET_0) time series produced by the different scenarios were compared. The analysis revealed that the output generated by scenario A is considerable higher than the ET_0 estimates generated by the other scenarios. It was found that the annual cumulative value of ET_0 from scenario A is on average approximately 200 mm larger than the annual value obtained from any of the other scenarios. The results produced by scenarios B and C are very similar in magnitude. Moreover, recommended ET_0 constraints [67] were considered to appreciate the performance of every scenario. Scenario A generates high estimates that violate these constraints by far. The opposite is observed for the output of the other scenarios as they are bracketed by the probability constraints.

To assess the impact of the method used for the estimation of time series of ET_p on the modeling of the hydrologic cycle, the MIKE SHE code [40] was applied to the basin of the Grote and Kleine Gete, using information of the weather stations Bierset and Ernage. The catchment is situated in the loamy region of Belgium and has a gauged size of nearly 585 km^2. The basin was subdivided in grids with a resolution of 600 x 600 m^2 [57]. The well known k_c-ET_0 method [3] was used to estimate ET_p time series. In the MIKE SHE code, the time series of ET_p are reduced to actual values using the Kristensen-Jensen model [94][40]. The study continued with the investigation of the effect of the different ET_p estimates on the model performance and the calibrated model parameters. To support this

analysis a Multi-Calibration (MC) test was implemented. In the MC test three models differing only in the ET_p input data were subjected to identical calibration and validation processes to obtain a unique comparison basis. In general, every model was calibrated by fit, in the period [01-Jan-1985, 31-Dec-1986] using a Split Sample (SS) procedure and a trial and error approach, against both daily catchment discharge measurements and observed water levels for 12 observation wells with filters in different geological layers. The SS validation period was defined as [01-Jan-1987, 31-Dec-1988]. To investigate how well internal variables were simulated, a Multi-Site (MS) validation test was performed. Also a Multi-Window (MW) validation test was implemented by considering windows with different amplitude. For the characterisation of the model performance and for optimisation purposes in general, use was made of the following statistical criteria: the Mean Absolute Error (MAE), the Relative Root Mean Squared Error (RRMSE), the coefficient of EFficiency (EF), and the Coefficient of Determination (CD). In addition, an Extreme Value Analysis (EVA) was performed in the period of available discharge observations (1984-1995) for assessing the quality of simulated peaks as a function of the ET_p scenarios. The Peak Over Threshold (POT) algorithm was used for selecting the independent peak events from the daily time series.

Paradoxically, in general, the model performance was better for the highest ET_p estimates (scenario A) than for the more appropriate estimates from scenarios B and C. Moreover, peaks were significantly underestimated in scenario A whilst they were overestimated in scenarios B and C. These facts seem to indicate that (*i*) discrepancies in terms of model performance are due to different antecedent moisture conditions that are in correspondence with the different ET_p scenarios; (*ii*) encouraging model performances may arise from wrong system descriptions; and (*iii*) there is an inadequate simulation of the runoff processes also due to the lumped daily time step adopted in the study. The differences among the sets of effective model parameters seem to be only marginal.

Application of information theory in the identification and calibration of watershed models

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Complex models for integrated watershed management pose questions about what can be known from limited available data. In any model development activity, a balance needs to be found between errors of bias and variance in the predictions made. Models that are too simple are incapable of reproducing the actual functioning of the system and too complex models may capture the structural behavior but mimic the noise in the data as well as. At the Center for Development Research, an integrated watershed model is being built to simulate the development of the Volta Basin in West Africa [162]. Of the eleven key-variables to be predicted, three are hydrological (*rainfall*, *evapotranspiration*, *river flow*) and two are related to water management (*water use*, *hydropower*). The remaining variables are socio-economical such as *population*, *income*, and *land use*. The idea is to simultaneously solve for all variables over space and time. The number of auxiliary variables and parameters is staggering with the SVAT-model alone accounting for 36 parameters.

The general consensus is that estimating all parameters and choosing a functional model architecture does not just pose major quantitative and computer logistical problems but also qualitative problems with respect to identifiability of parameters, given finite data sets. Common model development tools such as sensitivity analysis, cross-validation, and dimensional inspection may loose some of their power and new tools may be needed. One promising tool, on which I focus here, is information theory which has found useful applications outside its original field of electrical engineering in computer science, thermodynamics, economics, language processing, and, to a much lesser extent, hydrology (see for example [30]).

Information theory

The central quantity in information theory is entropy, H, which for a discrete random variable X with probability function $Pr(X = x) = p(x)$ for $x \in \chi$, is defined as:

$$H(X) = \sum_{x \in \chi} p(x) log\left[p(x)\right]$$

It is common to take the logarithm to base 2 in which case bits are the units of entropy. Without being a norm, entropy has some norm-like properties and is a measure of the information needed to describe the variable X. An important advantage of information theory is that it predicts probability properties without assuming particular probability functions or relations between variables. A simple least square regression finds the parameters that maximize the likelihood of the measured variables assuming those variables are

independently drawn from one normal distribution. An alternative approach is to assume as little as possible about the variables at hand which leads to maximum entropy methods, a variation of which has been applied in hydrology by [182].

Here, I focus on multi-variate entropy measures such as joint entropy, $H(X,Y)$, conditional entropy, $H(X|Y)$, and the mutual information of two variables, $I(X;Y)$, defined as:

$$I(X;Y) = \sum_x \sum_y p(x,y) log \left[\frac{p(x,y)}{p(x)p(y)} \right]$$

$I(X;Y)$ quantifies the information both variables have in common as which becomes clear if the above equation is re-written as:

$$I(X;Y) = H(X) - H(X|Y)$$

or in words: the mutual information is the reduction in entropy of one variable if the other variable is known. The mutual information equals zero when the two variables are completely independent. The usefulness is that, again, no particular functional relation between the variables needs to be assumed. In the example below, I exploit this to judge to what extent a particular rainfall/runoff model "distills" all available information from the rainfall record.

Finally, a remark concerning the Cramér-Rao inequality which sets an upper bound on the accuracy with which an unbiased probability function parameter can be calculated for a given set of variables drawn from that probability function [34]. In hydrology, an extension of this inequality has been used for minimum error estimation in inverse modeling of groundwater-flow [111]. Although no application is given here, it is of special interest in the sensitivity analysis of the integrated Volta watershed model because it shows that an increase in dimensionality of a system increases the variance of parameter estimates [66].

Example

The following (very) simple example shows how information theory can be used to identify the simplest model that expresses the bulk of the information contained in the independent variables. If we plot the yearly runoff (RO) against the yearly rainfall (P) for the Volta Basin from 1936 to 1964, when the river was dammed, we see a surprisingly good correlation. A simple linear regression gives RO=0.53(P-342) with r^2=0.80. A 3^{rd} order polynomial improves the fit to r^2=0.83, suggesting that higher dimensional models do not improve the predictions considerably. It would be possible, however, that some other function would still explain an important part of the remaining variability. Here, but especially in less straightforward cases where our priors on the physical plausibility of models are much weaker, it would be convenient if we could say in advance how much one variable set can tell about another. For the 1936-1963 Volta series, we can calculate H(P)=6.56, H(RO)=5.98, and H(RO,P)=9.20. The conditional entropy H(RO|P)=H(RO,P)-H(P)=2.64. This tells us that knowledge of the rainfall does indeed describe for an important part the entropy,

or information, of the runoff. For the normalized residuals of the linear model (Res), we have H(Res)=4.47, H(RO,Res)=9.92, and H(RO|Res)=5.45. With the conditional entropy almost being equal to the entropy of runoff, we can say that the residuals do not contain much information and that an increase in model complexity would not improve our predictions.

In the full paper, a more elaborated example will be given with a model for monthly runoff. The effect of the increased temporal resolution on information content will be shown. The results from cross-validations of models of increasing complexity will be compared to information-theory measures. Using Fano's [34], minimum prediction errors will be calculated. In conclusion, information theory does not tell us how to arrive at an optimal model but it tells us how optimal a model can possibly be and when we are getting close.

Uncertainty Quantification and Management of Model-Based Predictions for Complex Hydrological Systems

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Essential to the value of any predictive model of a physical system is the ability of making crisp statements about the confidence to be attached to its predictions. This confidence typically depends on a number of factors including **1)** the selection of the mathematical model representing the physical phenomena involved, **2)** the selection of a level of numerical effort to resolve the model in the presence of various environmental and structural constraints, **3)** the data going into calibrating the model and **4)** the data assimilation method used to integrate the data into the model. The first two of these factors, namely modeling error and numerical error,have received significant attention over the past several years, and methodologies for estimating the associated errors have been developed. The last of these factors, namely that associated with data assimilation, has witnessed a significant development over the past decade, mostly due to the significant growth in computing power, enabling data assimilation techniques to be implemented for systems at scales that are representative of the data collection efforts. A method is described here for the quantification of the third of the above factors, namely the sensitivity of the model predictions on the amount and quality of data with respect to which it has been calibrated. The ability to simultaneously quantify the errors associated with model selection,data, model calibration, and numerics opens the possibility for a rational allocation of resources among these four usually competing requirements, with the objective being a reduction of the overall prediction error. This will also permit an answer to each of the following two questions that are consistent with the level rigour of the model selection: **1)** given a particular model, a particular set of data, and a particular access to computational resources, what is the achievable level of confidence in the predictions from the model, and **2)** given a target level of confidence, what are the requisite resources in terms of data collection, analysis and computing.This sensitivity on data is clearly one significant source of uncertainty in the predictions. Controlling this sensitivity through data collection is a particular form of uncertainty management. The first step towards achieving the above stated goal consists of developing uncertainty propagation methodologies that allow the highlight, as part of their development, the explicit dependence of the predictions on the amount and quality of the data. Such a formulation would then allow the numerical evaluation of the required sensitivities. Such a method for uncertainty propagation has been developed based on a probabilistic representation of the uncertainty and relying on various spectral representations of stochastic processes, namely the Karhunen-Loeve expansion and the Polynomial Chaos expansion. These expansions together permit the representation of the predictions from numerical models as nonlinear surfaces in the uncertain parameters, with this representation depending explicitely on certain statistics of the data. The accuracy of these statistics clearly depends on the amount of data used in evaluating them, and

could therefore be used to gage the accuracy in the computed representation.The method is applied to a simplified cascaded model of a hydrological system consisting of catchment and a stream. The objective of the analysis is to identify data monitoring strategies aimed at increasing the reliability of the predictive model to within a specified tolerance.

5 Remote sensing and hydrological modeling
Chairman: R. A. Feddes

Assimilation of AMSR-E soil moisture retrievals into a land surface model

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It is widely believed that improved land surface states, such as soil moisture, surface temperature, and snow cover and properties, if assimilated into weather prediction models will result in improved forecasts. For the near future, the most promising satellite instrument for measuring soil moisture and snow properties is the Advanced Microwave Scanning Radiometer on NASA's Aqua spacecraft (AMSR-E). The AMSR-E validation plan recognizes the need to evaluate the derived level-2 and level 3 soil moisture and snow data products to assure that AMSR-E will provide products that are both accurate and appropriate for hydrological modeling and diagnostics studies. In addition, it needs to be demonstrated that the 25 km soil moisture data product is sufficiently accurate for applications such as assimilation. One major problem is the scale mismatch between the surface heterogeneity in soil wetness and vegetation and the 60 km AMSR-E footprint, which is interpolated to the 25 km gridded soil moisture product. In the paper we describe a simulation study to evaluate the AMSR-E gridded soil moisture data, which consists of: (i) high resolution modeling of the terrestrial water and energy balance, combined with a microwave emission model, to provide AMSR-E specific data at a modeling resolution of 1 km for the 560,000 km^2 Red-Arkansas River basins; (ii) simulation of the AMSR-E retrieval and gridding using the properties of the AMSR-E antenna gain function and Aqua orbit characteristics; and (iii) assimilation of the soil moisture back into a off-line macro-scale (25 km grid) hydrological model. The surface fluxes from the macro-scale model, with assimilated soil moisture, will be compared to the surface fluxes averaged up from the 1 km simulations.

Initialization of Soil Moisture in a Global Climate Model: A North American Case Study

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Accurate initialization and forecasting of land surface soil moisture in fully-coupled climate system models is critical for seasonal-to-interannual climatological and hydrological prediction. This results from the soil moisture feedback to precipitation and atmospheric circulations, through its control on partitioning of the available energy into latent and sensible heat exchange. To overcome such limitations in the NASA Seasonal-to-Interannual Prediction Project (NSIPP), a one-dimensional Kalman filter assimilation of near-surface soil moisture observations has been added to the Catchment-based Land Surface Model (CLSM) of [92, 46] used by NSIPP. In this paper, the CLSM is run off-line from the atmospheric and ocean simulation models, forced by bias corrected European Centre for Medium-Range Weather Forecasts (ECMWF) re-analysis data [10]. The atmospheric forcing data set, which extends from 1979 to 1993, includes four observations per day of the following fields; two meter air and dew point temperatures, ten meter wind speed, convective and total precipitation, long and short-wave downward radiation, and surface pressure. The CLSM is run off-line from the ocean and atmospheric simulation models so as to produce the best possible land surface initialization states from an optimal merging of the best possible land surface forecast using the best possible atmospheric forcing with remotely sensed observations of the land surface. To correct for soil moisture forecast errors resulting from incorrect initial conditions, inaccurate meteorological forcing data and an imperfect forecast model, remotely sensed measurements of near surface soil moisture are assimilated into the CLSM using a one-dimensional extended Kalman filter. The soil moisture estimates from the assimilation are compared with the limited number of ground-based point measurements of soil moisture. The near-surface soil moisture observations used in the assimilation are from the Scanning Multi-channel Microwave Radiometer (SMMR) satellite 6.6 GHz (C-band) channel covering the period 1979 to 1987 [116]. The soil moisture observations are derived simultaneously with the vegetation optical depth, by utilizing information in the Microwave Polarization Difference Index (MPDI) and a soil temperature estimate from the 37 GHz channel. The ground truth data for this time period is limited to 19 stations in Illinois, 6 stations in Iowa and a transect of 89 points in New Mexico [139].

Regional scale soil moisture assimilation in a NWP model using surface heating rates

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Introduction Changing climatologically prescribed soil moisture fields into prognostically evolving quantities in Numerical Weather Prediction (NWP) and climate models has led to considerable model drift problems in the recent past (e.g. [172]). The soil moisture reservoir has a relatively long timescale compared to other reservoirs in the hydrological cycle, and is therefore a likely candidate for sensing accumulated model errors. In operational NWP practice, drifts of this kind are usually avoided by assimilating observations in the model equations. Remotely sensed land surface characteristics gain interest in the fields of NWP and climate research, as they might contain information about the wetness of the surface and soil (see e.g. [143]). Various attempts to assimilate remote sensing land surface data in NWP model fields are reported in literature, both concerning passive microwave [85, 26] and thermal infrared observations [5, 6, 163]. As remote sensing observations become available at higher accuracy levels and spectral resolution, and as theoretical and technical development of assimilation of data in operational meteorological models evolves rapidly, major progress in this field is to be expected in due course.

A possibly valuable source of information is the surface heating rate after sunrise [175, 112]. The rate at which the land surface temperature changes is closely related to the surface evaporative fraction. Surface temperature observations using geostationary satellites may be used to control the soil moisture content in operational NWP models, as demonstrated in a limited number of case studies [5, 6, 83]. This paper describes a new case study, in which METEOSAT derived surface temperature measurements are assimilated in a NWP model for an area covering The Netherlands, Germany and parts of the UK. The main objective was to determine the potential use of METEOSAT or future MSG data for soil moisture assimilation under non(semi)arid conditions, such as present in the midlatitudes. Special attention is paid to the definition of the heating rate, cloud screening, atmospheric correction and data assimilation methodology. In the discussion the implementation of the system to construct a regional/continental scale data base of soil moisture content is discussed.

Heating rate definition The surface heating rate is defined as a change of surface temperature in time. However, a clear variation with time and location results from a strong effect of solar irradiation on surface temperature. A much stabler quantity is obtained when defining the heating rate as change of surface temperature per unit cos(solar zenith angle), or i. This variable appreciates the nearlinear dependence of surface temperature on surface available energy and net shortwave radiation. In order to reduce the effect of subtle nocturnal planetary boundary layer processes on the surface temperature immediately after sunrise, the heating rate is only computed for time slots with local time exceeding 2 hours after sunrise. Since the surface temperature generally shows an asymmetric response

over the day owing to the soil thermal inertia, only data earlier than 11 UTC local solar time are considered.

Cloud detection If clouds are absent, time series of thermal and visible radiances from METEOSAT are monotonically increasing (thermal radiance) or decreasing (shortwave reflectance). Pixels not obeying this expected behaviour are considered to be cloud contaminated. A refinement to this assumed monotonic and gradual change is developed here. A linear regression between surface temperature or reflectance as function of i is calculated, together with a statistical measure of the RMSdistance to this fit. Threshold values are defined to this RMSvalue, which indicate cloudcontaminated pixels when exceeded. Tuning and validation of the cloud screening procedure is carried out using synops data and operational cloud detection methods developed earlier at KNMI.

Atmospheric correction Earlier case studies exploring the use of observed surface heating rate for soil wetness indication usually ignored atmospheric corrections. However, for thermal satellite observations this correction is strongly correlated to surface temperature, and shows a pronounced diurnal cycle. Case studies have shown that the artificial heating rate resulting from ignoring the (time dependent) atmospheric correction may be as large or even exceeding the true signal in the surface heating rate observations. Therefore, atmospheric corrections are applied for a subsample of the pixels in the target domain, and spatial and temporal interpolation techniques are applied. This interpolation is necessary to reduce the requried computation time to a tolerable minimum.

Data assimilation procedure A number of simple dataassimilation methods was explored in order to detect whether METEOSAT data contained useful signal under midlatitude conditions. This signaldetection is considered to be more important than the design of a very sophisticated data assimilation system in the current stage of the research. The backbone of the data assimilation is the minimization of the difference between observed and modelled surface heating rates in the target domain. Surface heating rates were calculated by the land surface parameterization scheme in a NWP model, and are sensitive to changes in the soil moisture content in the model. The amount of soil moisture minimizing the difference to observations is considered to be the best estimate for the NWP model chosen. In order to be able to calculate surface heating rates that can be compared to satellite observations, a surface model is selected which explicitly calculated the temperature of an infinitesimally thin surface layer without heat capacity. This "skin layer" is able to respond nearly instantaneously to changes in radiation and surface fluxes. To calculate this skin temperature, the surface model of [172], later updated to a tiled version as described by [164] is used. Various minimization procedures were explored. The first method, labeled 'nudging', assumes a quasilinear relation between heating rate and soil moisture content. Initially two NWPsimulations are carried out, differing with respect to soil moisture content only. The difference in heating rate is then extrapolated to an assumed optimal soil moisture content, from which a third NWPsimulation is started. A new extrapolation leads to the final (fourth) soil moisture estimate, from which a 24hour forecast is started. For the next day, a new soil moisture assimilation is carried out for those pixels not contaminated with clouds. Limited data accuracy is accounted for by

reducing the final soil moisture increment proportionally to the relative number of valid METEOSAT pixels within the NWPgridbox. A more complex method uses a variational minimization procedure using a Newtonian root finding procedure. A cost function is defined in which the difference between modelled and observed heating rate is normalized by an assumed observation error. This observation error is again considered to be proportional to the number of valid METEOSAT pixels within the NWP grid box. An iterative root finding was applied, requiring a fairly large amount of NWP simulations (about 10 per assimilation cycle). A third simplified variational method is used combining the two methods described above. Again a cost function is defined, but its gradient is assumed to be linear near the final optimal model state. This reduced the required number of model integrations to N+ 1, with N the number of control variables (soil moisture layers) used to change the model state. When initialized without any prior knowledge of the soil moisture content the model can not be assumed to be close to the optimal state, and the assimilation was executed iteratively. However, at later times it is assumed that the model can not have diverged from the optimal state too far within the short simulation period since the previous assimilation cycle, and the assumption of a linear cost function gradient is applied.

Results Soil moisture fields on the (sub)continental scale are clearly difficult to validate against in situ measurements. Here an alternative validation is used by analysing modelled and observed relative humidity at screen level height (2m). Near surface relative humidity is closely related to surface evaporation, and thus a good indicator to detect the added value of the assimilation information. Relative humidity data were not used to estimate soil moisture contents and thus serve as a truly independent source of data. Two case studies were carried out, each compassing slightly less than a week. The periods were selected for having relatively large cloudfree areas in a significant portion of the simulation domain. The weeks are 27 May and 2629 June 1995. In the first week in May 1995, the control model (without soil moisture assimilation) showed persistent overestimation of relative humidity during daytime. Although a clear diurnal cycle was present (associated with uncertainties in the parameterization of boundary layer entrainment rather than surface flux errors), the soil assimilation reduced the average bias clearly when the nudging approach was used. The simplified variational assimilation displayed rather similar results. In the second period, a small underestimation of relative humidity was hardly affected by the soil moisture assimilation system. The systematic errors were clearly smaller than in the previous case in May, and the ability to repair these systematic errors were also less obvious. On the other hand, an expected reduction of the RMSerror of relative humidity predictions did not occur. It was expected that the high resolution data from METEOSAT (compared to the 50×50 km gridbox of the NWP model) would cause a better distribution of the soil moisture over the simulation domain, apparent from a reduction in RMS. This was not the case.

Discussion Using METEOSAT derived heating rates appears to bear possibility to improve on NWP forecasts of surface fluxes and soil moisture content, but there are a number of unresolved issues. First, the surface temperature as observed from METEOSAT is

clearly not only dependent on soil moisture content, but on any process that affects the skin temperature. Notably, aerodynamic cooling has a clear effect on skin temperature, and this is poorly resolved in most NWP models. In another data assimilation experiment, Van den Hurk et al. (2001) used a variational minimization procedure to control both the soil moisture content and a coefficient related to local aerodynamic coupling between the surface and the atmosphere. This combined optimization is probably feasible and necessary when using METEOSAT or MSG data to infer surface wetness conditions from surface temperature observations. Second, the case studies explored are not expected to show a strong impact of soil moisture on NWP forecast performance. Water supply is usually not limited during most of the year, and more significant contributions from satellite data can be expected in more (semi)arid environments. Third, the methodology is explored further in the context of generating a (sub)continental scale soil moisture estimate through NWP data assimilation. It is assumed that the combination of near surface synops observations and satellite data will reduce the number of degrees of freedom in an NWP model further, implying that the final model state matching all observations as close as possible will be of increased quality.

A Surface Energy Balance System (SEBS) for estimation of turbulent heat fluxes from point to continental scale

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A Surface Energy Balance System (SEBS) is proposed for the estimation of atmospheric turbulent fluxes and surface evaporation using satellite earth observation data in the visible, near infra-red, and thermal infrared frequency range, in combination with meteorological information at proper scales. SEBS consists of the following components:

1. a set of tools for the determination of the land surface physical parameters, such as albedo, emissivity, temperature, vegetation coverage etc. from spectral reflectance and radiance measurements [152, 102];
2. a model for the determination of the roughness length for heat transfer [153];
3. the BAS (Bulk Atmospheric Similarity) theory for the determination of friction velocity, sensible heat flux and the Obukhov stability length [22];
4. the concept of surface energy balance at limiting cases (dry and wet) for the determination of evaporative fraction.

SEBS requires inputs such as surface albedo, temperature, Planetary Boundary Layer (PBL) meteorological variables, and vegetation parameters (Leaf Area Index, Height, fractional cover) or land use and NDVI as a surrogate. The advantage of the system is that no a priori knowledge of heat fluxes is required and no site specific calibration is needed. Data of high or low spatial resolution from all sensors in the visible, near-infrared and thermal infrared frequency ranges can be used in the system. Based on a set of case studies, SEBS has proven to be capable to estimate turbulent heat fluxes and evaporation at scales ranging from a point to a continent with acceptable accuracy [101]. Nevertheless, further independent validations of SEBS with ground measurement data for complex surface types are still necessary in order to advance the understanding of the land surface processes.

Data assimilation framework for the estimation of surface fluxes and energy balance components using thermal remote sensing

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The estimation of surface energy balance and the exchange of mass and energy from land to atmosphere is required in many applications in hydrology and meteorology. In fact the fluxes determine soil hydrological status and act as a boundary condition for the dynamics of the troposphere. There are however no ground-based networks of surface flux and energy balance measurements that can provide fields of these variables across the global land regions. Remote sensing is the only viable approach to map these fields. The problem is that the spectral measurements from space-borne instruments are not directly linked to surface energy balance components and fluxes. The available measurements in microwave frequencies have a weak signal with respect to surface wetness since the dielectric constant properties of water are very different than that of soil minerals. Extraction of a surface wetness signal from the microwave measurements is hampered by surface roughness effects and the presence of even moderate vegetation. Thermal and visible remote sensing has a longer heritage and not only longer but more accurate and higher resolution data on surface thermal emissions are available from a number of platforms. The problem of visible and infrared measures is that they cannot be used in the presence of clouds or rain, thus limiting the use of such data for some monitoring applications like flood prevention. On the contrary, microwave brightness temperatures are not affected by clouds and rain, so they can be used with almost every meteorological conditions. Therefore, these measurements can be combined to form adequate data sets on the evolution of land surface temperature. What is needed is a physically-based framework for relating the land surface temperature and its evolution to the components of surface energy balance and surface fluxes. In the past approaches such as correlating vegetation indices and evaporation as well as thermal inertia techniques have been used. These approaches are mostly empirical and do not use the physical constraints afforded by modeling surface energy balance and soil heat diffusion. In this paper we introduce a data assimilation framework that uses the long heritage and current investments in thermal range remote sensing in order to produce data sets on surface energy balance components and surface fluxes. Given the complexity of the process, simplified models of surface energy balance and atmospheric boundary layer schematisations have to be applied. Furthermore, the physical quantities involved are usually not easy to measure, especially when dealing with medium or large scale problems. In this research, we use a model based on *force restore* approximation of the vertical heat diffusion equation, which gives the evolution in time of land surface temperature, in response to the forcing derived from energy balance at soil surface [38]. The forcing term is given by the balance of net surface radiation, latent heat flux and sensible heat

flux between earth and atmosphere. Such fluxes strongly depend on the one hand on soil moisture condition, on the other on the factors related to turbulent transfer mechanism at the earth surface (wind advection and surface aerodynamic properties). Previous studies [53] have shown the feasibility of determining a soil moisture index using an adjoint state variational data assimilation model, based on observations of land surface temperature and standard micrometeorological data.Here, the assimilation methodology developed in [53] is also extended to the determination of the factors related to turbulent transport and surface aerodynamic roughness characteristics.In most modeling applications, neutral conditions with a logarithmic wind profile are assumed, and the surface roughness factor is related to the land cover classification for the region, assigning an empirical value for each vegetation class. This can lead to serious errors in the estimation of surface fluxes. The present research follows a different approach, by-passing the problem of determining a priori empirical values of surface roughness. The influences of surface roughness, wind speed and near-surface atmospheric structure are grouped in a turbulent efficiency parameter, R which can be inferred again with a variational approach.The final objective is then to estimate simultaneously a soil moisture index α(or, more precisely, land surface control on evapotranspiration), the turbulent efficiency parameter R and the components of the surface energy balance related to these factors.The model is formulated in a way that once-per-day land surface temperature observations are sufficient, if taken near the hour of daily maximum [65], while the model time step can be arbitrary, depending on the availability of micrometeorological measurements (typically 3 hours).The model has been tested on the FIFE-site area, using the measurements made during the field campaigns held in 1987 and 1988 [141]. In a first phase, in order to test the model sensitivity, two experiments were made in the hypothesis of extreme values of soil moisture conditions. Thus, the model has been applied in case of a) complete soil saturation (maximum flux of latent heat for the given micrometeorological conditions), and b) when there is no flux of latent heat from the soil to the atmosphere. The results obtained give informations on the model's response in terms of roughness factor variations and on the effect of initial conditions. Other experiments were dedicated to the investigation of the model's numerical stability with different time steps.Another part of the research is focused on the evaluation of remote sensing techniques and their integration in the surface energy balance model. During the FIFE experiment land surface temperature was measured in the field, but when direct measurements are not available, as in most cases, remote sensing is the most suitable tool to obtain such data. Recent researches have adapted the model to the use of AVHRR infrared measurements [65]. Anyway, as previously stated, the use of infrared measurements is limited to non-cloudy situations. In order to obtain a more complete dataset, part of the present research was also dedicated to the development of a methodology for retrieving land surface temperatures from the Special Sensor Microwave/Imager (SSM/I), that measures microwaves emitted from earth surface at different frequencies and polarisation with a 25 km resolution. The results obtained have been compared with ground measurements made during field experiments like FIFE (Kansas, US, 1987 and 1988), HAPEX (Sahel, 1991-92) and from meteorological stations (meteo stations in ex-USSR, 1988-90), showing a good correlation.

Remote sensing estimates of rainfall surplus for catchment scale hydrological analysis

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The spatio-temporal patterns of rainfall surplus (rainfall minus actual evaporation) are key-information in catchment scale hydrology. These data can, however, not be straightforwardly obtained from standard weather stations because of two limitations:

(i) The spatial variability of rainfall surplus across a catchment cannot be described by point measurements. Moreover, (ii) actual evaporation differs often significantly from potential evaporation being the evaporation measure interpretable from routine weather stations. Remote sensing measurements can, however, help in interpreting point data and estimate the actual evaporation rate.

The results of weekly total rainfall estimated from 5 minute radar scans across The Netherlands will be presented. The Doppler type of a ground-radar of the KNMI is used for this purpose. There are a number of limitations of the technology, which will be discussed. It is proposed to include a dense rain gauge network to calibrate the radar backscatter signal. Geo-statistical procedures help in linking rain gauge data to the 2 km pixel scale backscatter coefficients of the radar.

Actual evaporation can nowadays be computed from the surface energy balance using low resolution satellite images from radiometers having visible, near-infrared and thermal infrared channels. Examples of NOAA-AVHRR data will be given. Low resolution images have the advantage of a short return period (1 or 2 days) which make them suitable for monitoring dynamic features such as land surface processes. The basic procedure is to compute the latent heat flux on cloud free days using the SEBAL model. The inverted Penman-Monteith equation is applied to obtain the surface resistance to evaporation for these days. In The Netherlands, some 25 good quality images can be retrieved in a year. For cloudy days, Penman-Monteith is used in the forward manner using routine weather data to account for a day-to-day variability of near-surface atmospheric conditions, with the surface resistance being taken from previous satellite tracks. The result is a 1 km grid of actual evaporation obtained under all weather conditions.

Daily and weekly rainfall surplus information can be used in catchment scale hydrological models. But also simple tree-decision models, which partition rainfall surplus into groundwater recharge and surface runoff, may be used. When recharge is known or can be ignored, runoff can be obtained as the water balance residual after including storage effects. Traditionally runoff is predicted from rainfall, but with information of actual evaporation from the satellite, it will be come feasible to compute runoff as the water balance residual term. This provides new avenues to determine local rainfall-runoff relationship which ultimately improves drainage design, flood protection actions, quantifying renewable water resources and the like.

Potential of ENVISAT ASAR observations for surface soil moisture retrieval

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In June 2001 a new Earth observation satellite will be launched by ESA. On board is an advanced synthetic aperture radar instrument, called ASAR. It is a C band (5.3 GHz) multipolarized sensor with different incidence angle capabilities and different spatial resolutions. This offers new possibilities for Earth observation and in particular for soil moisture mapping. This paper discusses the potential of ENVISAT ASAR observations for the retrieval of surface soil moisture for bare soils. The data set used in this study was obtained at the European Microwave Signature Laboratory (EMSL), Ispra, Italy, during a dedicated soil moisture experiment [108]. Using these data the accuracy of soil moisture retrieval based on an ASAR configuration and a surface scattering model is investigated. In particular the possibilities of using this soil moisture information for assimilation in distributed hydrological models is discussed.

Indirect estimation of soil moisture from energy balance

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In the earth-atmosphere system the mass of water is conserved at all times but it may be found in three different states (vapour, liquid and solid); it may be transported in a number of ways (including convection, precipitation, percolation and runoff); and this accumulation or depletion in stores is measured as change on water content (air humidity and soil moisture). In any given system at the earth's surface, evaporation is the connecting link between the water and the energy budget. Evaporation is in fact the common term in the water and energy balance equations and it plays a crucial role in governing the weather and climate. Air temperature and humidity are measure of thermal energy and water status of the atmosphere respectively that are strongly connected with the fundamental water and energy cycles of the land-atmosphere system. The complex land-atmosphere system may be then studied using the distribution of the principal climatological parameters (e.g. air temperature and relative humidity) in time and space, considering that such parameters are only indirect measures of more fundamental quantities. The knowledge of the radiative forcing namely solar radiation and the land-air temperature disequilibrium should implicitly contain information on the evaporation regime and the soil moisture conditions. Using a combination of a surface energy balance equation and an approximate expression of latent and sensible heat transfer, an application of a data assimilation system is here proposed and an index of soil moisture is estimated. Particularly an equation, as an indirect estimation method, is formulated regarding the soil relative humidity for net radiation, air properties and surface ground temperature. In a simple lumped system, when some secondary effects at the earth-atmosphere interface can be neglected, the energy balance equation can be expressed in terms of the specific flux of net incoming radiation equal to the sum of the specific flux of heat conducted into the earth, the latent and the sensible heat into the atmosphere, the rate of evaporation. Besides the net incoming radiation is composed of solar and thermal contributions, that are the downward longwave or atmospheric radiation and the upward longwave radiation and the (net) shortwave radiation, obtained from the global shortwave radiation considering the albedo of the surface. The longwave radiation, i.e. the radiant flux resulting from the emission of the atmosphere gases and the land and the water surfaces of the earth, can be expressed in terms of body temperature and emissivity. The upward longwave radiation is usually obtained by assuming that the ground is equivalent to an infinitely deep gray body of uniform temperature and emissivity, which is close to unit. The downward long-wave radiation under clear skies may be written using the air temperature near the ground (shelter level) and the atmospheric emissivity under clear sky, related to the dew point temperature, through the saturated vapor pressure. Approximate expressions of the latent and sensible heat fluxes

have been also used in the model, depending on gradient in temperature and specific humidity between the ground surface and the atmosphere. Particularly the latent heat flux parameterization has been related to the soil saturated specific humidity given by the integrated Clausius-Clapeyron relation on ground temperature and to an index α related to the relative soil saturation. The ground (soil) relative humidity obtained from the model described has then a functional dependence on conventional observation at meteorological surface stations, such as air and ground temperature, air humidity, pressure, wind speed and incoming solar radiation. The model has been preliminary tested considering the energy balance equation averaged over the diurnal cycle for which the heat ground flux has been assumed equal to zero. For the daily values of α estimated based on land-air temperature disequilibrium, a temporal analysis has been performed with the aim of analyzing the soil moisture time dynamics. Model's tests have been conducted using data from a few sites of the Oklahoma Mesonet [64], where all the required variables are measured. The daily values of parameter α for each of the mesonet locations has been estimated. Daily rainfall were used to roughly estimate the daily changes in soil moisture and from the experiments we can observe that the soil moisture index increases after a storm and decreases following the peaks after a storm. The model also correctly discriminates the periods where the evaporation regime is either energy limited and the part of inter-storm where the evaporation regime is water limited or soil/vegetation controlled. Others tests on the model's accuracy have been conducted using the automatic meteorological stations data sets from the 1987-1989 FIFE experiments [141] for which direct measurements of soil moisture are also available. Since in this tests the comparison among the few soil moisture data and the α-index are not satisfactory, a variational data assimilation approach has been also applied [53] including the surface energy balance in the estimation procedure as a physical constraint (the adjoint technique). Using standard surface micrometeorological data and the radiometric observations of ground temperature, this technique formulates the estimation problem as a minimization of ground temperature forecast errors. The surface energy balance equation is incorporated as a physical constraint and it has been represented by the force-restore equation, an ordinary differential equation in the soil surface temperature. The procedure yields estimates of latent and sensible heat fluxes as well as soil moisture time evolution $\alpha(t)$ that control the air saturation specific humidity at the ground surface. Comparison of estimated values of α and those based on FIFE observations are in very good agreement. Further tests will be conducted, in terms of spatial analysis, mapping α obtained for all the Oklahoma Mesonet Stations. The spatial patterns will be studied for a few rainstorm and those following long inter-storm, observing if the index responds to rainstorm and to the inter-storm dynamic (decay). The spatial distribution in soil water content could in fact include the local precipitation dynamics and the difference in water vapor evaporation that is affected by soil types and land use spatial variability. The maps of the time variation of α averaged over several days should also be correlated to soil type maps, since it is proportional to soil hydraulic conductivity and porosity depending by soil texture inhomogeneity. Correspondence between antecedent soil moisture and subsequent soil moisture anomalies will also be studied.

Estimation of surface energy balance components and surface control on evaporation: assimilation of ground temperature measured from satellite

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Satellite platforms provide a new and valuable source of remotely sensed data for land surface hydrology principally because of their spatial coverage. Since the remote sensing measurements are not direct observations of land surface hydrologic states and parameters, the retrieval is often an under-determined inverse problem. An emerging approach to solving such problems is data assimilation in which the synergy of multi-sensor/multi-platform (satellites as well as *in situ*) observations. Furthermore they can effectively impose dynamical constraints by using a model of the system as part of the statistical estimation.

In this paper a land data assimilation system is introduced that includes a system model constraint and a measurement component. Neither components are perfect, therefore noise and structured error are ascribed to each. The system is directed towards providing statistically optimal estimates of land surface turbulent flux (latent and sensible heat) and an index of land surface (moisture) control on evaporation based on merging the data assimilation components. Satellite remote sensing data from two low earth orbit platforms are used as the measurements.

Since land surface temperature estimates from satellite remote sensing are assimilated, the relevant system equation is heat diffusion equation at the surface and subsurface. Under the hypothesis that the soil thermal properties are nearly constant with depth and that the surface forcing term has a strong single-frequency (e.g. diurnal) component, the equation may be approximated by the so called force-restore equation [38, 79]. An aerodynamic resistance formulation is used to establish the surface turbulent flux rates. The aerodynamic resistance is based on a log-linear wind profile in the surface atmospheric layer with an aerodynamic roughness length scale z_0. This parameterization, valid for near-neutral conditions, reduces the number of terms depending on ground temperature, producing a slight degradation of the data assimilation system performance. There are however no obstacles to including stability correction except for the effort.

In the latent heat flux formulation, following [53], the specific humidity at the ground surface, q_g, is estimated by reducing the temperature-dependent saturation specific humidity (q^*)through a multiplicative and dimensionless index (α) which represents soil control on evaporation.

This formulation of the dynamic equation for surface temperature with energy balance, is

used in the model as a constraint on the estimation using adjoint technique.

Measurements of land surface temperature from satellite remote sensing are assimilated over two sub-regions within the Southern Great Plains 1997 hydrology field experiment in northeast Oklahoma. Two case studies are considered, each with a different input stream of measurements. In the first and ideal case that also serves as the reference for subsequent comparisons, half-hourly *in situ* ground temperature observations are the measurements in the data assimilation. In the second case satellite data from two low-earth orbit satellite are the only source of measurements for ground temperature.

Data from surface flux measuring stations and *in situ* soil moisture observations are used to validate the estimation results with ground-truth. It is shown that the data assimilation system performs well in capturing the day-to-day variations in the components of surface energy balance, ground temperature, and soil moisture or surface control on evaporation.

The performance of the estimation is linked also to the timing of the satellite over-pass. On days when satellite data are available close to the time of peak diurnal ground temperature, the estimation is considerably improved over days when the cumulative daily heating is unknown.

Assimilation of remotely-sensed snow observations in a catchment-based land surface model

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Snow plays an important role in governing both the global energy and water budgets, as a result of its high albedo, thermal properties, and being a medium-term water store. However, the problem of accurately forecasting snow in regional and global atmospheric and hydrologic models is difficult, as a result of snow related features that display variability at scales below those resolved by the models and errors in model forcing data. Hence, any Land Surface Model (LSM) snow initialization based on model spin-up will be affected by these errors. By assimilating snow observation products into the LSM the effects of these errors may be offset, but special care must be taken to avoid erroneous systematic influences on the water budget as a result of the assimilation.

To prevent artificial moisture transfer as a result of direct data insertion in the assimilation of snow, a one-dimensional Kalman filter assimilation of snow observations has been added to the Catchment-based Land Surface Model (CLSM) of [92, 46], used by NASA Seasonal-to-interannual Prediction Project (NSIPP). The CLSM uses the three-layer snow model of [106]. Our goal is to develop a snow assimilation scheme that optimally merges snow observations with the LSM forecast. This scheme takes into account the effects of snow melting as a result of bias in the LSM temperature. The snow assimilation scheme for updating of snow forecasts in the CLSM has been developed, using a version of the LSM that is un-coupled from the atmospheric and ocean models. Using an un-coupled LSM for an individual continent allows for development of a global snow assimilation scheme without the computational burden of a fully coupled global simulation. Moreover, this approach is consistent with the current soil moisture assimilation work being undertaken by NSIPP.

The snow assimilation algorithm is demonstrated in this paper through a series of identical-twin synthetic experiments, in which the same model used in the assimilation was used to generate the true states. A 20 year retrospective forcing data set for North America suitable for CLSM is used [10]. Special attention has been made to the updating of land surface and air temperature biases through the snow observation data, so that we may prevent erroneous snowmelt. This is a first step towards using SMMR and SSM/I satellite measurements of snow water equivalent and snow depth.

6 Data assimilation in hydrological modeling Chairman: P.A. Troch

Options for Hydrologic Data Assimilation: Matching the Method to the Problem

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Environmental data assimilation methods facilitate the interpretation of large amounts of diverse data, including non-traditional data obtained from remote-sensing. Most of these methods use models to enhance or improve the information provided by field measurements. Model-based data assimilation algorithms have the important advantage of being able to estimate variables which are not directly observable. Such algorithms have been used to map large-scale ocean and atmospheric circulation, to derive subsurface soil moisture profiles, and to locate petroleum reservoirs. In each case, models make it possible to estimate unobservable variables (e.g. subsurface soil moisture) from related observable quantities (e.g. microwave radiance). New remote sensing technologies and spatially distributed models offer great potential for improving our understanding of hydrologic processes, especially at large scales. Data assimilation will play a significant role in this enterprise. There is, however, much work to be done before operational data assimilation algorithms can be used to process all of the new data that will become available over the next few decades. In particular, we need to develop models and estimation approaches that are specifically designed to be used in data assimilation applications. These applications typically involve multiple data sources that observe different processes acting at different scales. The quantity of data to be processed will be much larger than has traditionally been the case in hydrology and much of this data will be of marginal value. Data assimilation algorithms must be sufficiently sophisticated to screen and interpret a continual stream of measurements in an efficient and physically meaningful way. This paper discusses some of the conceptual and design issues which hydrologists need to consider when applying data assimilation techniques. In particular, we examine some of the advantages and limitations of different approaches to data assimilation and we identify the methods that are most appropriate for particular problems. Methods to be discussed include variational assimilation, Kalman filtering (both traditional and ensemble filtering), multi-scale estimation, and heuristic techniques.

Soil moisture assimilation with the Ensemble Kalman filter in support of NASA's Seasonal-to-Interannual Prediction Project

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The goal of the NASA Seasonal-to-Interannual Prediction Project (NSIPP) is to develop the use of existing and planned remote sensing observation systems together with *in situ* data for improved predictions of seasonal-to-interannual climate variations. The prediction of precipitation over land at seasonal time scales is naturally a foremost objective of NSIPP. Seasonal climate forecasting must rely on the correct initialization of the slow components of the Earth system, namely, the land surface and the oceans. Although the ocean has the longer memory of the two, ocean conditions appear to have limited impact on predictability outside the tropics [51]. By contrast, the memory associated with the land surface, in particular soil moisture, is likely to be the chief source of mid-latitude forecast skill. Recent results [93] demonstrate the potential predictability of precipitation over land associated with soil moisture.

In this paper we examine the feasibility of using the Ensemble Kalman filter (EnKF) [49] for optimal soil moisture initialization. The EnKF is based on the propagation of an ensemble of model trajectories whose spread gives an estimate of the uncertainty of the soil moisture estimates. The forecast error covariances that are needed for the update are derived from the ensemble. The EnKF is an attractive option for land surface applications because 1) it is relatively easy to implement even if the land surface model and measurement equations include thresholds and other nonlinearities, 2) it is able to account for a wide range of possible model errors, 3) it provides information on the accuracy of its estimates, and 4) its sequential structure is convenient for processing remotely sensed measurements in real-time. On the other hand, the EnKF relies on a number of assumptions and approximations which may compromise its performance in certain situations. Most notably, the size of the ensemble is quite limited in large-scale applications.

In a series of synthetic (identical-twin) experiments we use the EnKF to assimilate near-surface soil moisture into the NSIPP Catchment Model of North America [92]. Ultimately, the goal is to assimilate directly L-band (1.4 GHz) and C-band (6.6 GHz) passive microwave brightness data. Our land model uses the hydrological catchment as the fundamental land surface unit. Within each catchment, the variability of soil moisture is related to characteristics of the topography. This modeled variability allows the partitioning of the catchment into several areas representing distinct hydrological regimes, wherein distinct (regime-specific) evaporation and runoff parameterizations are applied.

We assess the quality of the soil moisture estimates and the associated evapotranspiration

by comparing the estimates to the (synthetic) true fields as well as by examining the innovations sequence. The innovations are defined as the difference between the observations and the soil moisture forecast prior to the update. They are also available when actual observations are assimilated. The quality of the soil moisture estimates is mainly influenced by 1) the size of the ensemble, 2) nonlinearities in the hydrological model, 3) large-scale three-dimensional error correlations in the hydro-meteorological forcings, and 4) errors in the model formulation. Initial results indicate that the EnKF is a flexible and robust data assimilation option which gives satisfactory estimates even for moderate ensemble sizes.

On the improvement of discharge predictions through assimilation of ERS-based soil moisture data

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Over the past decade, a large number of methods to assimilate environmental state variables, such as soil moisture or surface temperature, into land-surface models, have been developed. These methods differ in computational efficiency, the degree to which the model relaxes towards the observations, the incorporation of errors in the observations and model results, and the need for spatial completeness of the observed data set. One unanswered question is whether lumped land-surface models can be improved to a similar degree as distributed land-surface models through data assimilation. This presentation focuses on the improvement of discharge predictions through assimilation of ERS-based remotely sensed soil moisture data. Data from the first (ERS1) and second (ERS2) satellite are used. ERS1 collected data from July 1991 through May 1996, and ERS2 since April 1995. During the overlapping period, an offset of exactly 24 hours was maintained between the two satellites. Both missions are characterized by a repeat cycle of 35 days, in which the orbit and position of the satellite over a specific area are identical. The nominal incidence angle is 23 degrees. Vertically polarized backscatter coefficients at C-band (wavelength 5.7 centimeter) are measured. The measured backscatter data for bare soils are inverted into soil moisture data by assuming that i) the soil roughness parameters do not change between two consecutive over-passes, and ii) the surface autocorrelation function has an exponential shape. By using a physically-based backscatter model (the Integral Equation, IEM, [62]) and an empirical backscatter model [121], and applying these two models for each pixel for two consecutive over-passes, a system with four equations (the Oh and the IEM model for the first and second overpass) and four unknowns (the dielectric constant for the first and second overpass, the soil root-mean-square height, and the surface correlation length) is obtained, for each pixel. This set of equations can then be solved for the soil roughness parameters and the dielectric constants. The dielectric constants are then converted into soil moisture values using the algorithm of [43]. The method was found to give good results for bare soil fields (a correlation of 0.86 with a root-mean-square error of 5.6% and a bias of 0.47% volumetric soil moisture were obtained). Because during the winter months (half October through half March) most of the catchment consists of bare soil, for which the described method can be applied, the study focuses on the assimilation of ERS-based soil moisture for the simulation of runoff-peaks during the winter. The hydrological model used is the TOPMODEL-based Land-Atmosphere Transfer Scheme (TOPLATS). The model was originally developed to simulate the surface water and energy balance for warm seasons [54], [126]. The hydrologic dynamics of the model has as its foundation the concept that shallow groundwater gradients set up spatial patterns of soil moisture that influence infiltration and runoff during storm events and evaporation and drainage in between storm events. The assumption is made that these gradients can

be estimated from local topography (through a soil-topographic index [145]). From this foundation, the model was expanded to include infiltration and resistance-based evaporation processes, a surface vegetation layer and a surface energy balance equation with an improved ground heat flux parameterization, and the effect of atmospheric stability on energy fluxes [54, 126]. More recently, winter processes (frozen ground and a snow pack), an improved water and energy balance scheme for open water bodies, and a two-layer vegetation parameterization were added [123]. Application to field experiments such as FIFE [126] and BOREAS [123, 124] have proven that the model can adequately simulate surface energy fluxes, soil temperatures, and soil moisture. The ERS-based soil moisture data are first assimilated into the distributed version of TOPLATS, using two different assimilation methods. Introducing the statistics of the ERS-data into the model, through the statistical correction assimilation method [76], leads to an improvement in the modeled discharge peaks. Assimilating the spatial structure and the statistics of the ERS-data, through nudging [150], leads to slightly better model results than the statistical correction assimilation method. Secondly, the ERS-data are assimilated into the lumped version of TOPLATS, again through the statistical correction assimilation method. The improvement in the modeled discharge peaks is similar as for the distributed model. As a consequence, it is suggested that it is sufficient to assimilate the statistics of remotely sensed soil moisture data into lumped hydrological models when one wants to improve hydrological model-based discharge predictions.

Assessing data assimilation of active microwave measurements along a transect hillslope through the Kalman filter

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We discuss the potential of retrieving information on the soil moisture profile from measurements of the surface soil moisture content through active microwave observations of the Earth. We use radar observations of the soil surface in a data assimilation framework to show that this allows the retrieval of the entire soil moisture profile. The data assimilation procedure under consideration is based on the Kalman filter technique. Kalman filtering allows the reconstruction of the state vector of a system when this system is represented by a dynamic model and when at least part of the state variables are observed regularly. The dynamic model of the system applied here consists of a finite difference implementation of the 2D Richards equation. The observation equation is based on the Integral Equation Model [62, 61] and is used to link the radar observations to surface soil moisture content. We evaluate this assimilation procedure through the application along a hillslope transect. Influence of system and observation noise, as well as the effects of the lateral relationships in the system model will be assessed.

Multi-scale data assimilation for predicting water fluxes in changing forest landscapes

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Land use changes over the last century have resulted in a mosaic of forest types in northern Wisconsin, USA. Continued forest management in the region present boundary definition problems for land surface hydrology modeling. We have developed a landscape scale coupled forest ecosystem - hydrology model that accounts for the role of changing forest cover types on land surface - atmosphere water flux. The model uses a multi-level canopy with half-hourly time steps for physiologically based calculations. Model calibration and validation was made using a combination of field, flux tower and remotely sensed observations, representing multiple scales of observations and spatial data inputs to drive the model. Ground-level measurements included sap-flux, micrometeorology, leaf area index, and net primary productivity. We made continuous measurement of transpiration in four cover types, red pine, sugar maple/basswood, quaking aspen/balsam fir, and northern white-cedar/balsam fir/alder, using Granier-type and Kucera-type sap-flux sensors from June through September, 2000, with a second field season to follow in 2001. The four cover types represent 90 percent of the basal area and 80 percent of the ground area within the footprint area of the WLEF AmeriFlux Tower. The other 20 percent consists of mostly non-forested areas, including grassland, shrub land and water. The four instrumented forest cover types represent functional prototypes for calibrating the model. Model calibration was performed using a multi-criteria Monte Carlo calibration technique, where the criteria include coefficient of variation, RMSE, and bias. Parameters were selected for calibration through a multi-stage analysis and refinement. The major parameters selected related to maximum stomatal conductance, sensitivity of stomatal control to vapor pressure deficit, aerodynamic properties of the canopy, soil moisture dynamics, and light interception. Transpiration from each of the stand types and their respective 7 dominant forest species were simulated with inputs of half-hourly micrometeorological measurements. Daily predictions of stand level transpiration explained from 64 percent to 92 percent of the variance of the daily measured transpiration, with some species showing tradeoffs between maximizing variance explained and minimizing bias. To further understand these tradeoff, a cluster analysis was performed on the sub-optimal to near optimal parameter-model combinations, which revealed physiologically significant correlations between parameters. The most significant correlation was a strong relationship between maximum stomatal conductance and sensitivity of stomatal conductance in well-coupled canopes, such as the red pine. Sensitivities to different parameters varied among species types, demonstrating that the key to modeling water fluxes in the evolving managed forests requires a detailed knowledge of species types. The sensitivity analysis also showed significant model prediction changes depending upon the vertical placement of the micrometeorological measurements (e.g., in canopy, below canopy, or above canopy at the WLEF tower). These differences also manifested themselves differently among species,

owing to the different canopy architectures.The forest cover prototypes were then used to parameterize the landscape scale model. A detailed remotely sensed forest cover classification was developed using airborne multispectral imagery. A detailed ground survey of leaf area index was developed using a cyclical multi-scale sampling scheme. The landscape level simulations of daily transpiration fluxes were compared with eddy covariance data collected at the WLEF tower. The WLEF tower showed a dominant vapor pressure deficit (VPD) control on total evapotranspiration from the region, with a linear relationship between flux and VPD. Alternatively, the model predictions of transpiration showed asymptotic relationships at higher levels of VPD owing to the importance of stomatal closure. However, the tower flux during wetter soil periods was equivalent to the lower end of modeled transpiration, and the dry period tower flux was approximately equal to the upper end transpiration. The model predictions reveal that landscape level patterns of water flux may be significantly regulated by forest physiological control, particularly during dry periods when there is little surface water. This result is important because current forest management practices in the region are promoting an increase in aspen and other fast growing species, which have lower water use efficiencies than their conifer and northern hardwoods counterparts.

Assimilation of surface soil moisture data for root zone soil moisture predictions in hydrological modeling

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The exchange of heat and moisture between the land surface and the atmosphere impacts the dynamics and thermodynamics of the weather and climate systems. The states of the surface and root zone soil moisture reservoirs are key variables controlling surface water and energy balances. For instance, in distributed hydrologic models the antecedent soil moisture conditions significantly influence flood amplitudes. Generally, there is a need for accurate spatial and temporal representation of soil moisture in models of hydrologic (flood forecasting, irrigation and agriculture) and atmospheric processes. In response to this, Soil-Vegetation-Atmosphere-Transfer (SVAT) models have been developed to simulate these mass and energy transfers, and to correctly determine soil moisture conditions from the solution of moisture and energy balance equations.The accuracy of the land surface flux estimates is potentially limited by the accuracy of the root zone soil moisture predictions. Emerging efforts in data assimilation seek to guide models with periodic observations of certain state variables, such as surface soil moisture. Any structural bias that may exist in the predicted soil moisture variables will limit the utility of the data-model merger.We present progress on important questions in SVAT modeling to achieve maximal benefits of the data assimilation. We adopt the force-restore SVAT model, which is a popular land surface model, used extensively in meteorological and hydrological modeling and also useful for soil moisture assimilation for its parsimonious parameterization and modeling of a surface soil layer of about 10 cm and a total root zone layer. We describe a simple approach for correctly predicting surface soil moisture in the case of stratified soils with a marked vertical inhomogeneity. We then present a new approach to update the root zone soil moisture in the SVAT models from information extracted from periodic observation of the near surface soil moisture, such as may be given by remote sensed observations. We report improvements in root zone soil moisture predictions using an operational assimilation system that on a daily frequency updates the measured surface soil moisture and root zone soil water content through a derived analytical treatment of the time rate of change of surface soil moisture, in a manner that compensates for both inaccurate initial conditions and model parameter estimates. A common limit of state variable updating procedures is that their efficacy may be limited by model calibration. When the model parameters are far from optimal there is need for a parameter updating procedure, which dynamically adjusts the parameters. Some doubts exist on the reliability of the parameter adjustments over such a short interval of time as the observation interval. More attractive and reasonable is the updating of physical parameters over a larger time

scale, in light of persistent model bias. For this reason, the proposed assimilation protocol also updates, at longer time interval, one of the most significant model parameters, the saturated hydraulic conductivity, deriving a quantitative estimate of the required adjustment from the governing dynamic equations.The combined framework is a multi-scale assimilation protocol that updates at short time scale (e.g. daily) the observed surface soil moisture and at long time scale (e.g. monthly) model physical parameters.The approach is successful tested on data collected during a pair of field experiments, where a site in Virginia (USA) provides evidence of dynamics under dry conditions and a site in Cork (Ireland) captures dynamics under wet conditions.The new approach can be successfully applied in distributed hydrologic modeling at different spatial scale, allowing an efficient simulation of heat and moisture exchange between the land surface and the atmosphere, but, at the same time, a parsimonious model physical parameterization, a reasonable skill and low computational efforts.

Data assimilation in groundwater modeling using Kalman filtering

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Groundwater modeling is an area where data assimilation is an important element for improving the predictive capabilities of the model. Information on the water and its environment is sparse, difficult to access, and most of all relatively imprecise especially because of heterogeneities in the soil. In most of the recent research, data assimilation schemes have been applied only in fairly simple groundwater models where the computational burden was not an issue. A scheme like Kalman filtering, which requires a large quantity of runs of the model, could be used without the need of excessive computational time. One of the most comprehensive data assimilation schemes is the Kalman filter. In its original version, however, it can be used only in linear systems, such as saturated zone modeling with constant hydraulic conductivities and specific storage. For more complex problems where non-linearities cannot be neglected and the state of the system is high-dimensional, Kalman filter schemes have been introduced that significantly reduce the computational needs linked to the covariance matrix calculations. Two such schemes are the reduced rank square root Kalman filter (RRSQRT KF) [170] and the ensemble Kalman filter (EnKF) [49]. The RRSQRT filter uses a lower rank approximation of the square root of the covariance matrix and a model linearisation to calculate the Kalman gain. On the other hand, the EnKF relies on Monte Carlo simulations and the full dynamics of the model to evaluate the covariance matrix. Both of these schemes have already been used successfully in other computer demanding domains, like coastal area modeling using a 2D hydrodynamic model. This study aims at assessing the utility of Kalman filtering in two different kinds of groundwater models: a fairly simple finite difference groundwater model and the integrated modeling system MIKE SHE developed by DHI Water Environment. Two applications of the Kalman filter are studied: error correction and parameter estimation. In the case of the simple finite difference model, the scheme is applied for correction of the piezometric heads and estimation of hydraulic conductivities. In the case of MIKE SHE, the scheme is extended to correction of catchment runoff and estimation of surface water flow parameters.The two models are compared with respect to both the efficiency of the data assimilation scheme and the computational needs. In the case of the simple model, data assimilation is used extensively to compensate for the simplicity of the model. On the other hand, the computational burden for running MIKE SHE does not allow for a large amount of runs, limiting the possibility of using complex data assimilation schemes. Nevertheless, being a more sophisticated model, MIKE SHE should provide more precise results that would need smaller corrections. Conclusions will be drawn on the use of data assimilation in integrated models in cases where data are sparse and may not provide sufficient information for precise parameter estimation.

Improving REW-scale modeling (POWER model) by 4-dimensional data assimilation techniques

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In recent publications by Reggiani et al. [134, 133], a wholly new framework for modeling the relation between rainfall and runoff at the watershed scale has been presented. Within this framework, a catchment is subdivided into a number of spatial entities that are termed *Representative Elementary Watersheds* (REWs). The set of REWs forming the entire watershed resembles a Strahler order channel network structure. Each REW may be interpreted as a volumetric computational unit or element. An REW comprises five characteristic zones for modeling the hydrological catchment behaviour. These zones are: 1) *unsaturated zone*, 2) *saturated zone*, 3) *saturated overland flow*, 4) *concentrated overland flow*, and 5)*river channel*. Watershed-scale conservation equations are derived for each zone of REW. They constitute a set of *Ordinary Differential Equations* (ODEs) that, combined with some topological relationships, can be solved to calculate characteristic hydrological state variables of REWs. The set of governing equations have been incorporated in a numerical rainfall-runoff model called POWER (stands for Planner-Oriented WatERshed-scale model).

The use of REWs for watershed modeling is very appealing since, compared to fully distributed physically-based approaches such as Mike-SHE and IHDM, the number of required catchment parameters remains limited. Moreover, model parameter values and state variables of each zone are defined at the spatial scale of the REW. Values of some model parameters should be obtained from field measurements and some others have to be obtained indirectly. In the REW-approach parameter values must be optimised during the model calibration stage. In distributed physically-based runoff models, however, parameter values are often modified by a trial-and-error procedures in which they are manually modified in order to simulate the measured state variables as good as possible. In runoff modeling, mostly the channel flow hydrograph is used as (the only) calibration variable although efforts have been reported on the use of groundwater level and/or soil moisture data as well. The use of multiple state variables as groundwater level, soil moisture, and hydrograph data in the process of model calibration is questionable due to the different temporal and spatial scales they exhibit. In this work, the potential of 4-dimensional data assimilation (4DDA) techniques for improving the performance of POWER is investigated by use of multiple state variables.

Data assimilation can be seen as an automated, efficient, state estimation procedure that can be used to improve model performance. Applications of data assimilation are often

reported in oceanography and meteorology while the application in hydrology is still under investigation. McLaughlin [110] presented an overview of data assimilation in hydrology. Most applications in hydrology are reported in the field of saturated and unsaturated flow. For the latter, in addition to field measurements of soil moisture contents, remote sensing is often used. The use of 4DDA in rainfall-runoff modeling has not received much attention. This is partly due to the fact that many runoff codes apply a lumped conceptual model structure and as such do not calculate the state variables in a spatially-distributed manner.

It is believed that the performance of POWER model in runoff forecasting can be significantly improved by use of 4DDA. Since the number of state variables to be calculated in POWER is limited, the state vector and the observation vector can remain small. This allows for computationally optimal state estimation. During forecasting, selected state variables must be updated when additional measurements become available. The discrepancy between calculated and measured state variables will serve to condition the state estimation problem. In this study, an extended Kalman filter will be used to optimise the objective function. It is foreseen that data on the groundwater levels and channel runoff will be used. The Geer basin (a tributary of Meuse River in Belgium) is selected as a test site.

Newtonian nudging for a Richards equation-based finite element model of coupled overland and subsurface flow

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New data sources for observation of hydrological processes can alleviate some of the problems facing the validation and operational use of hydrological models. Data assimilation provides a means of integrating these data in a consistent manner with model predictions. We will describe the implementation of a relatively simple data assimilation technique in a relatively complex hydrological model. The assimilation technique is Newtonian relaxation or nudging, in which model variables are driven towards observations by adding to the model equations an additional "forcing term" which is proportional to the difference between simulation and observation. Interpolation in space and extrapolation in time is done via 4D weighting functions that can incorporate some prior knowledge about the spatial and temporal variability and characteristic scales of the state variable(s) being assimilated. The numerical model couples a 3D finite element Richards' equation solver for variably saturated porous media and a DEM-based finite difference diffusion wave approximation for surface water dynamics. Coupling is via interaction between surface ponding heads generated by the subsurface model, computed as the residual between potential and actual atmospheric inputs (rainfall and evaporation), and the overland accumulation (in lakes and reservoirs) or routing (on hillslopes and in channels) of this ponded water.

The Darcy, Richards, and convection-diffusion equations that form the basis of the coupled model are widely accepted mathematical representations of verifiable conservation principles, so this physically-based distributed model, capable of reproducing the spatial and temporal patterns of pressure head, soil moisture content, saturation, and other variables, is a good candidate for data assimilation. The tradeoff, however, is that owing to parameterization and computational complexities the model is not practically applicable at large scales (we restrict our attention to hillslope and sub-catchment flow processes), and the more sophisticated data assimilation techniques will only compound these difficulties. Nudging appears to be a suitable scheme for conducting some initial investigations into the applicability and effectiveness of data assimilation for Richards equation- based 3D hydrological models. We will examine some of these issues, and will address in particular the numerical and physical performance of the assimilation model, including its impact on mass conservation, numerical stability, and nonlinear convergence.

Progress and Challenges in Operational Land Surface Data Assimilation

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Subsurface moisture and temperature stores exhibit persistence on seasonal-to-interannual time scales. This persistence has important implications for the extended prediction of climate and hydrologic extremes. However, errors in forcing, parameterization, and physics accumulate in modeled land surface stores, which leads to future errors in water and energy partitioning. This has motivated the development of land surface data assimilation methods, which constrain land surface simulation models by forcing them primarily by observations, and by using observations of land-surface storages to realistically constrain model evolution using data assimilation techniques. This development: (1) improves understanding of the time and space variability of hydrological and energy budgets, (2) mitigates land surface parameterization and observation errors through continuous simulation-observation inter-comparison, and (3) improves the initialization and dynamics of land surface states in numerical weather prediction models, for more realistic weather and climate predictions. An overview of past and current multi-scale hydrologic data assimilation research will be presented, with an emphasis on the unique challenges the land surface poses for data assimilation tools. Further, a review of future needs in operational land surface data assimilation will be offered.

Accurate initialization of land surface moisture and energy stores in weather and climate system models is critical for extended atmospheric and hydrologic prediction because of their regulation of surface water and energy fluxes between the surface and atmosphere over a variety of time scales [142]. Soil moisture, temperature, and snow exhibit persistence on seasonal-to-interannual time scales; together with external forcing and internal land surface dynamics, this persistence has important implications for the extended prediction of climatic and hydrologic extremes [91]. Because soil moisture, temperature, and snow are integrated states, errors in land surface forcing and parameterization accumulate in these stores, which leads to incorrect surface water and energy partitioning.

However, new high-resolution land surface observations are becoming available that will provide the additional information necessary to constrain land surface predictions at multiple scales. These constraints can be imposed in two ways. Firstly, by forcing the land surface primarily by observations (such as precipitation and radiation), the often severe atmospheric numerical weather prediction land surface forcing biases can be avoided. Secondly, by employing innovative land surface data assimilation techniques, observations of land surface storages such as soil temperature and moisture can be used to constrain unrealistic simulated storages. These land data assimilation systems also have the ability to maximize the utility of limited land surface observations by propagating their information throughout the land system to unmeasured times and locations. Data assimilation is a scientific tool that can not only lead to better predictions, but also helps to diagnose

model weaknesses and suggests where better parameterization is needed. The fusion of modeling and observations via data assimilation requires access to large volumes of surface atmospheric and hydrologic variables, usually in near-real time.

Significant progress has been made in land-surface observation and modeling at a wide range of scales. Projects such as the International Satellite Land Surface Climatology Project (ISLSCP), the Global Soil Wetness Project (GSWP), and the GEWEX Continental-Scale International Project (GCIP), among others have paved the way for the development of operational Land Data Assimilation Systems (LDAS). The development of LDAS serves as an integrating linkage between a variety of Earth science disciplines and geographical locations. But most importantly, LDAS integrates state-of-the-art modeling and observation on a operational basis to provide consistent high quality land states in a timely enough manner to be used in real-time applications.

The observational emphasis of LDAS is to assimilate spatially-distributed observations (i.e. remotely sensed observations) of the land surface that will provide memory to land-atmosphere interaction. Remote observations of interest include temperature, soil moisture (surface moisture content, surface saturation, total water storage), other surface water bodies (lakes, wetlands, large rivers) and snow (areal extent, snow water equivalent).

Recent advances in understanding soil-water dynamics, plant physiology, micrometeorology, and the hydrology that control biosphere-atmosphere interactions have spurred the development of Land Surface Models (LSMs), whose aim is to represent simply yet realistically the transfer of mass, energy, and momentum between a vegetated surface and the atmosphere. LSM predictions are regular in time and space, but these predictions are influenced by model structure, errors in input variables and model parameters, and inadequate treatment of sub-grid scale spatial variability. Consequently, LSM predictions of land surface hydrology and land surface states will likely be much improved by the assimilation strategies.

There are many different approaches to land surface prediction, which has lead to great diversity in LSMs. Several recent LSMs are currently used in LDAS, including the Mosaic LSM of [90], the National Centers for Environmental Prediction (NCEP), Oregon State University (OSU), United States Air Force (USAF), and Office of Hydrology (OH), LSM, called NOAH, the Variable Infiltration Capacity (VIC) model of [104] and the recently emerging Common Land Model (CLM).

Charney et al. [28] first suggested combining current and past data in an explicit dynamical model, using the model's prognostic equations to provide time continuity and dynamic coupling amongst the fields. This concept has evolved into a family of techniques known as four-dimensional data assimilation (4DDA). "Assimilation is the process of finding the model representation which is most consistent with the observations" [105]. In essence, data assimilation merges a range of diverse data fields with a model prediction to provide that model with the best estimate of the current state of the natural environment so that it can then make more accurate predictions. The application of data assimilation in hydrology has been limited to a few one-dimensional, largely theoretical studies

[48, 114] primarily due to the lack of sufficient spatially-distributed hydrologic observations [110]. However, the feasibility of synthesizing distributed fields of soil moisture by the novel application of 4DDA applied in a hydrological model was demonstrated by [76]. Six Push Broom Microwave Radiometer (PBMR) images gathered over the USDA-ARS Walnut Gulch Experimental Watershed in southeast Arizona were assimilated into the TOPLATS hydrological model using several alternative assimilation procedures. Modification of traditional assimilation methods was required to use these high density PBMR observations. The images were found to contain horizontal correlations with length scales of several tens of kilometers, thus allowing information to be advected beyond the area of the image. Information on surface soil moisture was also assimilated into the subsurface using knowledge of the surface-subsurface correlation. Newtonian nudging assimilation procedures were found to be preferable to other techniques because they nearly preserve the observed patterns within the sampled region, but also yield plausible patterns in unmeasured regions, and allow information to be advected in time.

The characterization of the spatial and temporal variability of water and energy cycles is critical for the improvement of our understanding of land surface-atmosphere interaction and the impact of land surface processes on climate extremes. Because accurate knowledge of these processes and of their variability is important for climate predictions, most NWP centers have incorporated land surface schemes into their models. However, errors in the NWP forcing accumulate in the surface and energy stores, leading to incorrect surface water and energy partitioning and adversely affecting related processes. This has motivated the NWP centers to impose ad hoc corrections to the land surface states to prevent this drift. Land Data Assimilation Schemes (LDAS), which are uncoupled land surface schemes that are forced primarily by observations, and are therefore not affected by NWP forcing biases are currently under development. This research is being implemented in near real time using existing LSMs by NCEP, NASA, Princeton University, Rutgers University, the University of Maryland, and the University of Washington at a 1/8th' (about 10 kilometer) resolution across the United States to evaluate these critical science questions. The LDAS are forced with real time output from numerical prediction models, satellite data, and radar precipitation measurements. Model parameters are derived from the high-resolution EROS vegetation coverages.

A real-time LDAS system is currently in place (see http://ldas.gsfc.nasa.gov), that uses near-real time NCEP Eta model analysis fields, along with observed precipitation and radiation fields to force several different land surface models in an uncoupled mode. Forcing, parameter, resolution, and prediction specifications for this North-American LDAS were carefully chosen by the inter-institution LDAS working group.

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