Impact of uncertainties in modelling soil water on recharge estimates

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Executive summary

Quantifying the evaporative losses and the changes in soil water content to an acceptable accuracy is a critical component of estimating groundwater recharge using a water balance approach. In particular, the soil water store plays an important role in moderating the evaporative losses during periods of low rainfall coinciding with high evaporative demand, with a consequent impact on the timing and quantity of recharge. Therefore, we have focussed on investigating the uncertainties arising from using different soil water numerical models.

There are three sources of uncertainty in the soil water model, i.e. the FAO56 soil water model that will be used by the Environment Agency:

- The model structure;
- The model parameters;
- The driving variables.

Uncertainties in the model structure have been investigated by comparing the output of the FAO56 soil water model with those from other models. Comparing the simulated model output with the historical observations has allowed us to assess the uncertainties due to the parameter estimation. The uncertainties in the driving variables have not been assessed in this study.

The study is confined to a land cover of grass, partly to minimise uncertainties arising from variations in the vegetation cover and partly because data for this land cover is significantly more available than for other types.

Uncertainties due to the structure of the FAO56 and Four Root Layer (FRL) soil water models were assessed by firstly calibrating the model's available soil water content by driving them with measured rainfall and evaporation and minimising the root mean square error (RMSE) of the difference between the simulated soil water contents and measured values, using a Monte-Carlo approach to generate the parameter values. The driving variables and measured soil water contents were from two sites located on the Berkshire Downs as part of the LOCAR programme. The soil water models were then driven with the measured evaporation replaced by Penman-Monteith potential evaporation and the process repeated to calibrate the remaining parameter values. The RMSEs achieved using the FAO56 soil water model were higher than those with the FRL. This is attributed to the latter's ability to simulate the changes in soil water content due to rainfall events, when a soil water deficit was present, in a more realistic manner.

The uncertainties due to parameter values were investigated by using defined parameter values. The available soil water content was derived from the NSRI's data whilst the values for other parameters were taken from the literature about the models.. Both soil water models were driven using observed rainfall and Penman-Monteith potential evaporation, calculated from measured meteorological variables, for the two LOCAR sites, which had fairly short time series, and four sites which had long term measurements. Neither soil water model was able to simulate the soil water deficits, during winter months, of chalk soils well. There was no consistent difference in the RMSEs achieved with the two soil water models when all the sites were considered, suggesting that the uncertainties, due to variability in the available soil water content between the sites and the "average" value used, were more significant than those due to the differences in the structures of the two soil water models.

A sensitivity analysis of the two soil water models was carried out by generating 50,000 parameter sets using a Monte-Carlo procedure, and calculating the RMSE between the simulated and observed soil water deficits. The results show that the available soil water content was the most significant parameter for both soil water models. The soil water models' simulations were relatively insensitive to the values of other parameters but essentially the same RMSE could be achieved with a variety of parameter sets.

A soil water model based on unsaturated flow was used to simulate the soil water deficits measured at one of the LOCAR sites on the Berkshire Downs. A significantly lower RMSE was obtained, compared to the other two soil water models. This was probably mainly due to the improved ability to simulate the slow drainage of the soil, particularly during the winter months. This gain is at the cost of significantly greater model complexity and computational time.

A brief summary of recent research studies into the hydraulic properties of chalk soils and the unsaturated zone is given. These have shown that flow through the matrix is the dominant flow mechanism and, where fracture flow occurs, it is likely to account for between 17 and 32% of annual recharge. The studies have shown that drainage through the unsaturated zone occurs throughout the year, albeit it at varying rates. A very important conclusion is that the top portion of the profile, ca 0.8 m, plays a major role in modifying the surface inputs, of water and solutes.

The conclusions of this study are:

- The model structure of the FAO56 soil water model results in greater uncertainties in simulated soil water deficits than are achieved with the FRL soil water model;
- The model structure of the FRL soil water model allows it to simulate the development of soil water deficits more successfully than the FAO 56 sol water model;
- Neither the FAO56 not the FRL soil water models simulate slow drainage of the soils, a feature particularly apparent during the winter months;
- Both soil water models are most sensitive to the value of the available soil water parameter and relatively insensitive to the other parameter values
- Both soil water models can produce simulations of soil water deficit with relatively similar uncertainties with a range of parameter sets;
- Uncertainties due to the value of the available water content are greater than those due to the differences in the soil water model structures;
- There is very little information available about the variability in the fractional available soil water of a soil series or of the rooting depth of a vegetation type;
- The use of a soil water model based on the Richards' equations of unsaturated flow, such as used in MOSES, provides a better description of drainage than those based on the capacity approach, but this is at the cost of a significant increase in computational time and the number of model parameters;
- Recent research has demonstrated the importance of matrix flow in the unsaturated chalk and constrained the range of flow through fissures;
- Recent research has demonstrated the importance of the upper part of the profile, ca 0.8 m, of chalk soils in attenuating the inputs.

Contents

1 Introduction

Quantifying the evaporative losses and the changes in soil water content to an acceptable accuracy is a critical component of estimating groundwater recharge using a water balance approach. In particular, the soil water store plays an important role in moderating the evaporative losses during periods of low rainfall coinciding with high evaporative demand, with a consequent impact on the timing and quantity of recharge. Therefore, we have focussed on investigating the uncertainties arising from using different soil water models.

There are three sources of uncertainty in the soil water model, i.e. the FAO56 soil water model, that will be used by the Environment Agency:

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Uncertainties in the model structure have been investigated by comparing the output of the FAO56 soil water model with those from other models. Comparing the simulated model output with the historical observations has allowed us to assess the uncertainties due to the parameter estimation. The uncertainties in the driving variables have not been assessed in this study.

2 The soil water models

The FAO56 soil water model (Allen *et al*., 1998) has been compared with the FRL (Four Root Layer) soil water model (Ragab *et al*., 1997). A brief resume of the models is given here whilst a full descriptions can be found in Chapter 7.

Both models are based on the capacity approach, i.e. they use a simple balance of the soil water content and implicitly assume that flow of water can occur through the store within the time step of the model (in most applications this is one day). Thus the change in the soil water content, during a given time step, is a balance between increases due to the effective precipitation, *W*, (this includes snow melt but actual precipitation is reduced by interception, i.e. water/snow held on the vegetation canopy and evaporated directly back into the atmosphere without passing through the soil) and reductions due to evaporation, *E*, (i.e. transpiration from plants and direct evaporation from the soil). When the volumetric soil water content exceeds a given threshold, θ_f, (the field capacity) the excess is considered to flow out of the soil store (i.e. drainage). A second threshold is defined as the volumetric soil water content at which evaporation ceases, θ_w, (the wilting point). A further threshold (the critical soil water content) is defined as the volumetric soil water content, above which evaporation is not limited by the availability of soil water, θ_d. The evaporation is reduced, by a linear function, between the critical and wilting point soil water contents. The major difference between the FAO56 and FRL soil water models is that the former deals with this as a single store whilst the latter considers that the soil water zone is divided up into four vertical layers of equal thickness. This leads to an additional parameter for the FRL model – the fraction of roots in each layer.

It should be noted that the volumetric soil water contents described above are defined as the soil water contents per unit volume of the soil. In order to determine the mass (and thus the “depth”) of the soil water the zone over which the changes in the soil water content are being considered must be defined (and thus is a model parameter). This is referred to as the rooting depth (units are of length). As might be expected from its name, it varies with the type of vegetation being considered but it is not necessarily the “true” rooting depth of the vegetation but the maximum soil depth within which evaporative losses occur, as such it includes a zone beneath the true maximum rooting depth, from which water can be drawn upwards as capillary flow, i.e. in response to the high water suctions developed within the zone of soil water deficits. As such, the rooting depth is also a function of the soil type. For many types of soil this additional thickness can be considered, for practical purposes, as being the same. However, there are some soils for which this could lead to an uncertainty which would be significant. A good example of this is chalk soil where soil water deficits have been observed to depths significantly greater, several metres, than the assumed rooting depth.

3 The measurement sites

The study has been limited to sites where the land cover is grass. This is mainly because it reduces uncertainties arising from the vegetation canopy having significant differences through the seasons but it also reflects the availability of data.

A full description of the calibration and quality control procedures and, if appropriate, the methods used to derive variables from measurements is given in Chapter 8

3.1 Short term measurements

Measurements made during the Lowland Catchment Research (LOCAR) programme from two sites in the Pang and Lambourn catchments have been used, Table 3.1. These measurements began early in 2003 and so only cover a short period. However, they have the virtue of including measurements of evaporation which can be used either as input to the soil water model, or to test the simulated actual evaporation.

Table 3.1 Measurement sites on grass in the Pang/Lambourn catchments used in this study

LOCAR number	Location	Grid Reference	Soil/geology	Date measurements began
PL16	Highfield Farm	SU 539703	Wickham series/London Clay Formation	Dec 2002
PL21	Sheepdrove Farm	SU 359815	Andover Series/Chalk	Jan 2003

The soils at the two sites are very different. At Sheepdrove Farm they are typical of the chalk with a thin, about 0.2 m, superficial layer, including a significant fraction of flints, overlying weathered chalk which grades into unweathered chalk between 1 and 3 m depth. In contrast the soils at Highfield Farm consist of a fine loam down to about 0.4 m, below which the sequence is dominantly clay with horizons containing varying amounts of gravel.

Care must be used when considering the results based on the measurements from Highfield Farm as, during the process of quality control and analysis of the soil water measurements, it became clear that there were significant differences in the soil water measurements from the four neutron probe access tubes, suggesting marked horizontal heterogeneity. Without additional data it is not possible to be absolutely certain as to why this is but a preliminary hypothesis is that there is a local perched water table present, associated with a gravely horizon. This was unexpected given that the site is on a hill top. Despite this, the decision was made to use these data as the perched water table appears to be between 0.5 and 2 m in depth and so the average water content from the four tubes would be consistent with the measured evaporation which will be the average conditions over horizontal distances of many 10s of meters.

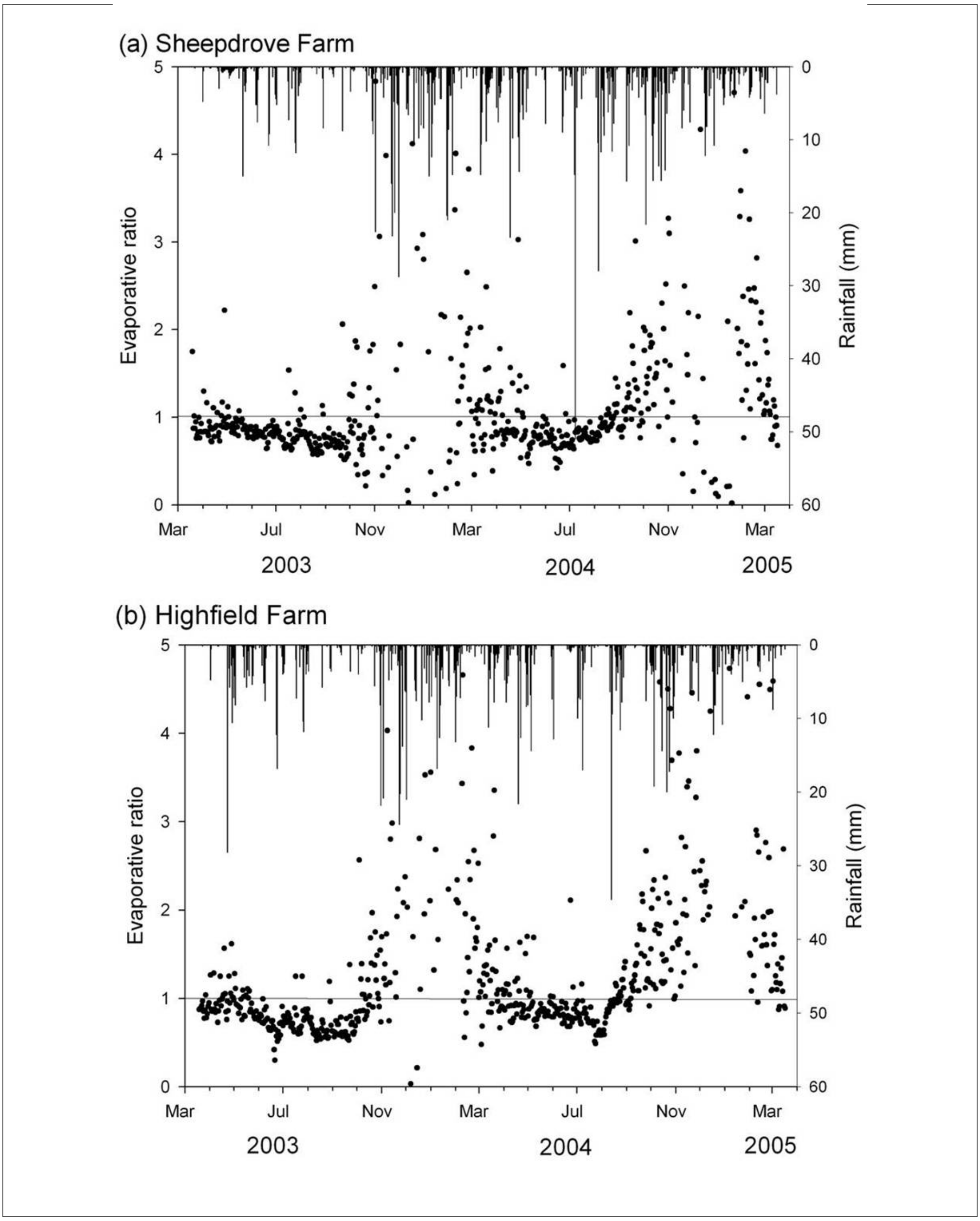

Figure 3.1 Time series graphs of evaporative ratios and rainfall at (a)Sheepdrove Farm and (b) Highfield Farm

A useful method of investigating the impact of soil water stress is to calculate the evaporative ratio, the net radiation divided by the latent heat flux (the latent heat flux is the evaporation multiplied by the latent heat of vaporisation). This is based on the premise that the evaporation rate is dominantly driven by the net radiation. In the UK, the value will generally be around 0.9 in the absence of a sizeable soil water deficit. There is considerable variability, particularly during winter, due to the advective component (dominantly driven by wind speed, humidity and air temperature) of the latent heat flux. Another component of the variability results from changes in the nature of the land surface but this tends to be on a longer term than the driving variables.

Time series graphs of the evaporative ratios at the two sites are shown in Figure 3.1. The data from Sheepdrove Farm suggest that a period of evaporation limited by soil water stress began in early July 203 and went through until early October 2003, broken for a short period at the end of August. The evidence for a period of soil water stress during the summer of 2004 is ambiguous. A similar pattern can be seen in the data from Highfield Farm, but the period of soil water stress during 2003 is longer and the effect of the lack of rainfall more marked. At this site there is a period, late August and early September 2004 when the evaporation is again reduced by soil water stress. Thus these data contain information that can be used to investigate the effect of soil water deficits on evaporation.

Soil water contents were measured using two methods: neutron probe and Profile Probes. Neutron probes are a well established method and allow measurements to be made to significant depths (4 m in this study) at intervals between of 0.1 and 0.3 m. The major disadvantage is that it is a manual system and so it is not possible to obtain data at high temporal resolution. The period between measurements was about 2 weeks. These data are complimented by measurements from Profile Probes; a new instrument that can be data logged at short time periods (15 minutes in this study). However, measurements are made at six, fixed depths down to 1 m. Data from both these instruments are available at Sheepdrove Farm but, at Highfield Farm, the heterogeneity of the soils and problems with instrument mean that no useful data from the Profile Probes is available.

There is an automatic weather station (AWS) at Sheepdrove Farm which provides hourly measurements which include the driving variables needed for evaporation models (rainfall, the components of net radiation, soil heat flux, relative humidity, air temperature and wind speed). At Highfield Farm a raingauge provides measurements of 15 minute totals.

3.2 Long term measurements

The long term measurements are from sites that have been used in previous studies. Two of the sites are on Chalk and two on the Sherwood Sandstones. Given the anticipated difficulties of soil water models simulating the soil water contents of chalk soils there is a focus on this aquifer. A summary is given in Table 3.2.

Table 3.2 Long-term soil water monitoring sites

Site	Grid reference	Geology	Average Annual rainfall (mm)	Monitoring	
				Period	Frequency
Bridgets Farm	SU 517337	Upper Chalk	798	1976-81	2 week^{-1}
Fleam Dyke	TL 549549	Middle Chalk	550	1978-83	5 week^{-1}
Bicton College	SY 075862	Sherwood Sandstones	800	1988-92	1 week^{-1}
Bacon Hall	SJ 652237	Sherwood Sandstones	625	1987-91	1 month^{-1}

At all these sites the soil water contents were measured using neutron probes. The driving variables, for an evaporation model, were from the nearest meteorological station whose data is held in the Met. Office's database of daily manual measurements. The measurements were in the form of minimum and maximum air temperatures, wind run, relative humidity or wet and dry bulb temperatures and sunshine hours. The latter were used to calculate the net radiation using mainly the method given by Thompson *et al*. 1981.

4 Assessment of uncertainties

The analysis has been carried out using computer programs written in FORTRAN. The FRL and MOSES soil water models were already available and so only the FAO56 model needed to be coded. Additional code was written to read in the driving variables and parameter values, calculate the objective function, carry out any analysis required and output the results.

In the following analyses, the root mean square error, RMSE, has been used as the objective function because it is widely used as a measure of both systematic and non-systematic differences. The RMSE was calculated as:

$$RMSE = \sqrt{\frac{\sum_{1}^{n}\left(O_i - S_i\right)^2}{n}}$$

where n is the number of measurements, $O_{,i}$ is the ith observed variable and S_i is the corresponding simulated variable. In this study the observed variable is the measured soil water deficits, θ-θ_f, and the simulated variable is the soil water deficit simulated using the soil water models.

4.1 Model structure

A number of studies, e.g. Finch and Harding (1998) have demonstrated that measurements of evaporation made using the eddy covariance method can be relied upon, at least in the case of short vegetation. The availability of such measurements of evaporation, from sites in the Pang/Lambourn LOCAR catchments, gives the opportunity to test the simulations made by soil water models, against observations, in isolation from models of evaporation. As a result, the uncertainties due to the structure and parameter values of the evaporation model are eliminated. There remain uncertainties associated with the measurements of the driving variables, rainfall and evaporation, but these are probably less than the uncertainties of the driving variables of the evaporation model: rainfall, net radiation, wind speed, air temperature and humidity.

Thus, it has been possible to explore the uncertainties in model structure by comparing the simulated values of the two different soil water models: FAO56 and FRL (see Chapter 8 for full descriptions of these models). In order to allow the uncertainties due to the model structure to be isolated from those due to the parameter values, the soil water model parameter values were calibrated using the observed soil water deficits. This was achieved by firstly calculating the total soil water deficits in the top 1 m of the soil profile. There were a number of reasons for choosing a depth of 1m for the total soil water content:

- A depth of 1 m is generally taken as the “rooting depth” of grass and is the value given in the data obtained from Cranfield University by the Environment Agency;
- Inspection of the measured soil water contents showed that the soil water deficits were dominantly within this zone;
- Soil hydraulic properties are generally available for the soil zone and do not extend into the underlying bedrock and the depth of the transition between soil and bedrock tends to be of the order of 1 m depth.

In the case of Sheepdrove Farm, the data from the Profile Probes were used and the measurements were aggregated with depth by using the depth interval weighted means of the six measurements. The results of this were then aggregated with time to give daily mean values. For Highfield Farm the data from the neutron probes were used and so it was only necessary to aggregate the readings for depth.

A Monte-Carlo procedure was used to calibrate the soil water model parameters by generating 50,000 parameter sets at random, with the parameters constrained to be within bounds that were physically possible, e.g. the values for the critical volumetric soil water were set to be greater than the volumetric soil water content at wilting point and less than that at field capacity. Both the soil water models use a parameter that is available water content expressed as depth of water, i.e. the volumetric soil water content multiplied by the rooting depth. Hence varying both the rooting depth and the volumetric soil water content does not produce any additional information in this study which is not considering differences in the vegetation type. Therefore the rooting depth was set to a constant value of 1 m (as will be used in the Agency's methodology for a land cover of grass), whilst the volumetric available water content was varied.

The calibration procedure was a two stage process. Because the measured evaporation includes the effect of soil water stress, the first stage was to calibrate the value of the available soil water content by driving the soil water models with the measured evaporation and the measured rainfall. The soil water stress factor was set to 1 (i.e. the volumetric water content at which soil water stress begins to effect the evaporation rate was set to the same value as volumetric water content at wilting point). However, it was still necessary to calculate the stress factor, at least in the case of the FRL soil water model, in order to allocate the actual evaporation to the appropriate model layer. In the second stage the remaining soil water model parameters were calibrated by using the calibrated value of the available soil water content and driving the models with the measured rainfall and Penman-Monteith potential evaporation (PE), the latter calculated from the meteorological measurements. The use of Penman-Monteith PE in place of the measured evaporation for periods without soil water stress introduces additional uncertainties but other studies (e.g. Finch and Harding, 1998) suggest that these are likely to be small. It should be noted that this is an ill-posed problem because there are more parameters, two for the FAO56 model and three in the case of the FRL model, than there are observed variables.

The model runs cover the period 1 January 2003 to 17 March 2005 and were initialized with the measured soil water content, interpolated to 1 January 2003. The soil water models were run with a daily time step and so the driving variables (rainfall, measured evaporation and PE) were aggregated to daily totals.

The resulting parameter values and the RMSE values are given in Table 4.1. At both sites, the RMSE values for the soil water deficits simulated by the FRL soil water model are lower than those for the values simulated by the FAO56 soil water model. These results show that, for these measurements at these sites, the uncertainties due to model structure are less for the FRL model than the FAO56 model. Thus the additional complexity of the FRL soil water model does result in an improved ability to simulate the soil water deficits. The parameter values obtained lie within the range that can be reasonably expected, with the exception of the soil water stress threshold for Highfield Farm which seems surprisingly low – the implication is that evaporation is reduced in the presence of virtually any soil water deficit. This may be as a result of the heterogeneity in the subsurface conditions at this site, i.e. that the soil water measurements were made at locations that are wetter than is generally the case for the zone that dominates the measured evaporation. Thus, the low value for the threshold is required to reduce the evaporation in the spring and autumn.

Table 4.1 Comparison of uncertainties using calibrated soil water model parameters

Site	Soil water model	Available water content (mm) $(\theta_f-\theta_w)z$	Soil water stress threshold $(\theta_f-\theta_d)/(\theta_f-\theta_w)$	Root density (m) Z_{65}	RMSE
Sheepdrove Farm	FAO56	107	0.21		26.5
	FRL	214	0.10	0.282	18.1
Highfield Farm	FAO56	262	0.86		19.1
	FRL	315	0.08	0.146	16.6

A greater understanding of the potential impact on estimates of groundwater recharge can be gained by considering the time series plots of the simulated and observed soil water deficits. For the Sheepdrove Farm site, Figure 4.1, the uncertainties in the simulated soil water contents from both models are essentially the same during the winter months and are due to the divergence of the assumption made by the models that drainage to a defined soil water content, field capacity, occurs within a day. The texture of the chalk is such that there is no such well defined level (Wellings, 1984).

During the remainder of the years, the soil water contents simulated by the FRL soil water model are in better agreement with observations, than those from the FAO56 model, except during September and October 2004. This is as a result of wetting up of the soil profile during the first half of August. Consequently, the timing of the elimination of soil water deficits, simulated by the FAO56 soil water model, is in closer agreement with the observations than that by the FRL model. However, this could be an artefact due to the rainfall data from Sheepdrove Farm being missing for the 6th to the 10th August. These data were infilled with those from Highfield Farm, multiplied by a constant factor determined by linear regression between measurements at the two sites. From the time of year and the intensity and duration of the dominant rainfall event, it is likely that the rainfall was due to convectional systems and so with greater spatial variability making the infilling more subject to error. If less reliance is placed on the results from this period then the FRL soil water model predicts the period without soil water deficits, and thus when recharge could occur, slightly better than the FAO56 soil water model.

A feature of the FRL soil water model, compared to the FAO56, is its ability to represent increased evaporation rates associated with rainfall events during periods of soil water deficits. Good examples of this can be seen in the simulated soil water deficits in August and September 2003. Wetting up due to rainfall events is more rapidly eliminated in the simulation with the FRL soil water model.

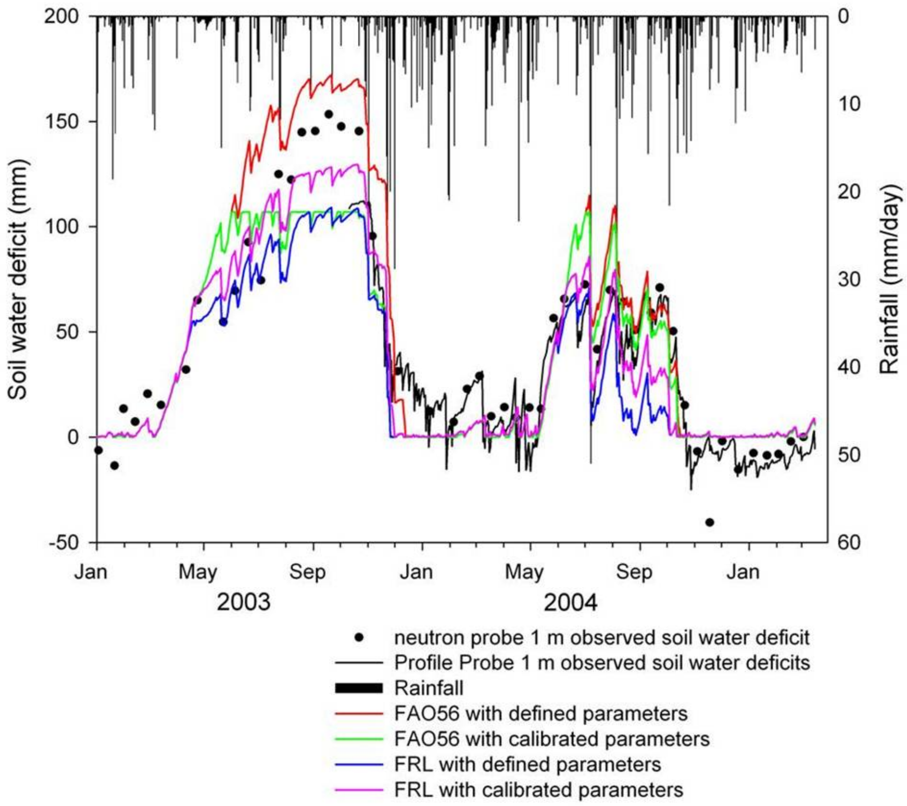

Figure 4.1 Simulated and observed soil water deficits at Sheepdrove Farm

The results for the data from Highfield Farm are not quite as conclusive because, although the RMSE obtained using the FRL soil water model is better than that from the FAO56 model, Table 4.1, the difference is quite small. An examination of the time series plots of observed and simulated soil water deficits, Figure 4.2, shows that this is because the FAO56 soil water model simulates the soil water deficits at the height of the 2003 summer well, whilst the FRL soil water model performs better at other times when soil water deficits are present. There is comparatively little difference, about 10 days, between the simulated periods of soil water deficits so that the impact on estimates of recharge are likely to be small. The values for the soil water stress threshold parameter in the two models are totally different and it is unclear why this is so. The effect is that the FAO56 soil water model will be unconstrained by soil water stress (and hence its ability to simulate the large soil water deficits observed in the summer of 2003) whilst the FRL soil water model will reduce the evaporation and thus the drying out of the soils more markedly. If a perched water table is present in parts of the site then this might be a more realistic condition.

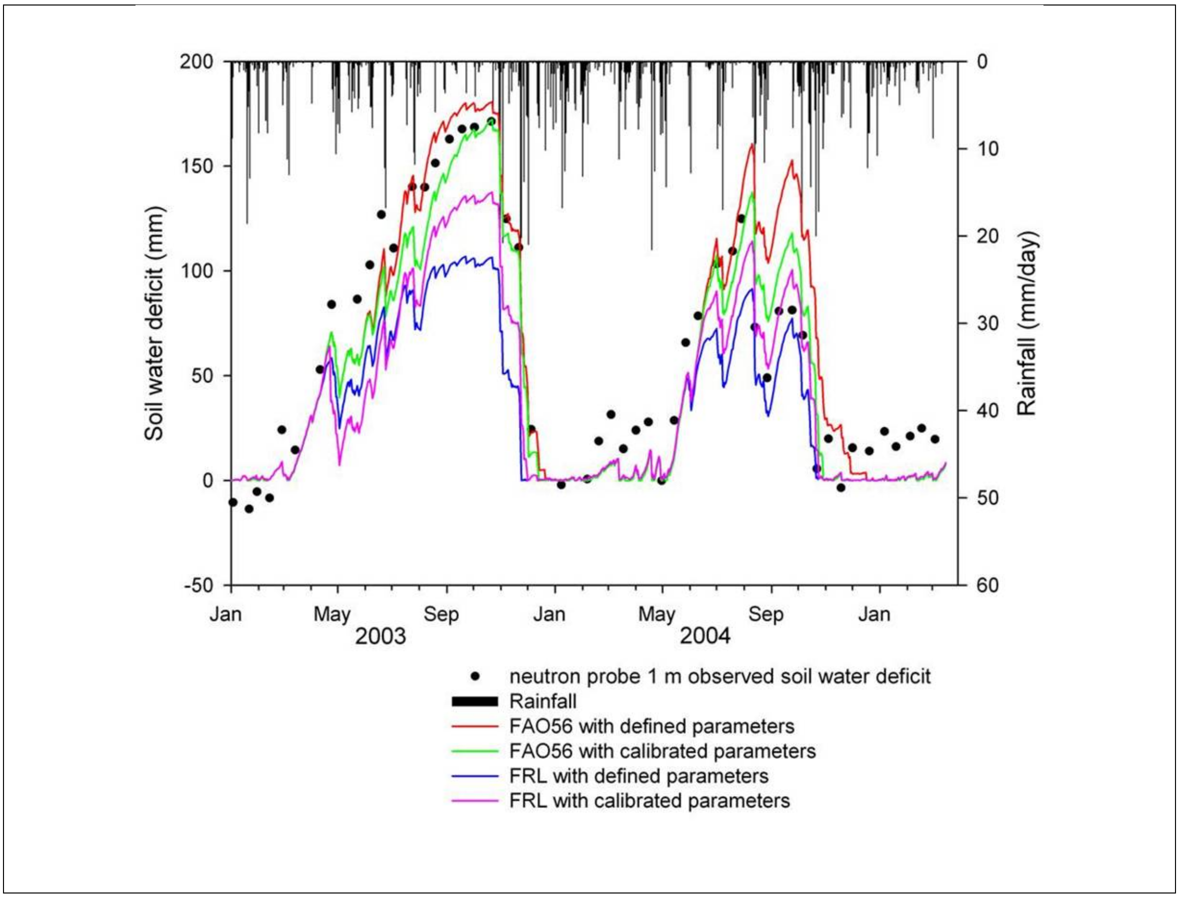

Figure 4.2 Simulated and observed soil water deficits at Highfield Farm

4.2 Model parameters

The uncertainties due to the soil water model parameters has been investigated by focussing on the available soil water content by using defined values. These were from the information available to the Environment Agency from the National Soil Resource Institute (NSRI) by aggregating the parameters for the soil layers and the bedrock as the thickness weighted mean values. The critical soil water content was defined using the recommended value given by Allen *et al*. (1998) whilst the root proportion parameter for the FRL soil water model was taken from Gerwitz and Page (1975)

4.2.1 Short term measurements

The RMSEs for the simulated soil water deficits, using the defined parameter values, are larger than those when using the calibrated parameter values, Table 4.2, as would be expected. The differences are significantly greater in the case of the data from Highfield Farm than those from Sheepdrove Farm. An examination of the time series of simulated values of soil water deficits for Sheepdrove Farm, Figure 4.1, shows that the FAO56 soil water model with the defined parameters performs poorly during the summer of 2003 due to the low available water content. For the remainder of the simulation it does not perform significantly differently to the same model with the calibrated parameters. In comparison, there is a greater difference between the values simulated by the FRL soil water model with the two parameter sets. The main reason for this is again the lower available water content with the NSRI parameters but the effect is consistent through most of the periods when soil water deficits are present.

This reflects the different ways that the two models handle the impact of soil water stress. The use of four layers with different root proportions in the FRL model means that soil water stress begins to reduce the actual evaporation at lower soil water deficits than the FAO56 model (see Ragab *et al*., 1997). In effect, to simulate the same level of soil water deficits, the FRL soil water model needs a high value for the available water content than does the FAO56.

Table 4.2 Comparison of uncertainties using defined soil water parameters at short term measurement sites

Site	Soil water model	Available water content (mm) $(\theta_f-\theta_w)z$	Soil water stress threshold $(\theta_f-\theta_d)/(\theta_f-\theta_w)$	Root density (m) Z_{65}	RMSE
Sheepdrove Farm	FAO56	183	0.4		28.8
	FRL	183	0.5	0.163	25.5
Highfield Farm	FAO56	194	0.4		26.0
	FRL	194	0.5	0.163	36.2

A similar situation occurs with the data from Highfield Farm, Figure 4.2. However, it is clear that the value for the available water content from the NSRI's data is very inappropriate when used with the FRL soil water model. However, given the concerns about the heterogeneity of the soils at this site, it is unclear how typical these conditions are of this soil series. Whereas, at Sheepdrove Farm much more confidence can be given that the soils are representative of chalk soils of the region because these soils are more homogeneous.

4.2.2 Long term measurements

The model runs were initialised by "spinning up" the soil water models with a year's driving variables data.

For both the chalk sites, Bridgets Farm and Fleam Dyke, the defined parameters and those obtained by calibrating the soil water models have been tested.

The values for the RMSEs obtained with the data from Bridgets Farm, Table 4.3 suggest that the FAO56 soil water model with the defined parameters gives the best simulation of the soil water deficits. However, an examination of the time series, Figure 4.3, shows that this is because this combination simulates the extreme conditions of 1976 best. The results are not as good in subsequent years. If the RMSEs are recalculated ignoring the data for 1976 then the values for all four combinations of sol water model and parameter sets are virtually indistinguishable. Using the calibrated parameters, the simulated soil water deficits by the FRL and FAO56 soil water models are very similar, although the FRL model does tend to simulate the detail of the largest soil water deficits better. None of the model/parameter combinations simulate the wet conditions of 1981 well. As commented above in Section 4.2.1, none of the models are able to simulate the soil water conditions well at chalk sites during the winter months. This reinforces the hypothesis that the basis of these models, i.e. the capacity approach, is not compatible with the hydraulic conditions in chalk soils.

Table 4.3 Comparison of uncertainties at long term measurement sites

Site	Soil water model	Available water content (mm) $(\theta_f-\theta_w)z$	RMSE
Bridgets Farm	FAO56 (defined)	183	42.9
	FAO56 (calibrated)	107	48.2
	FRL (defined)	183	52.7
	FRL (calibrated)	214	49.9
Fleam Dyke	FAO56 (defined)	183	33.9
	FAO56 (calibrated)	107	31.3
	FRL (defined)	183	34.8
	FRL (calibrated)	214	30.8
Bicton	FAO56	109	29.5
	FRL	109	27.1
Bacon Hall	FAO56	126	29.6
	FRL	126	49.2

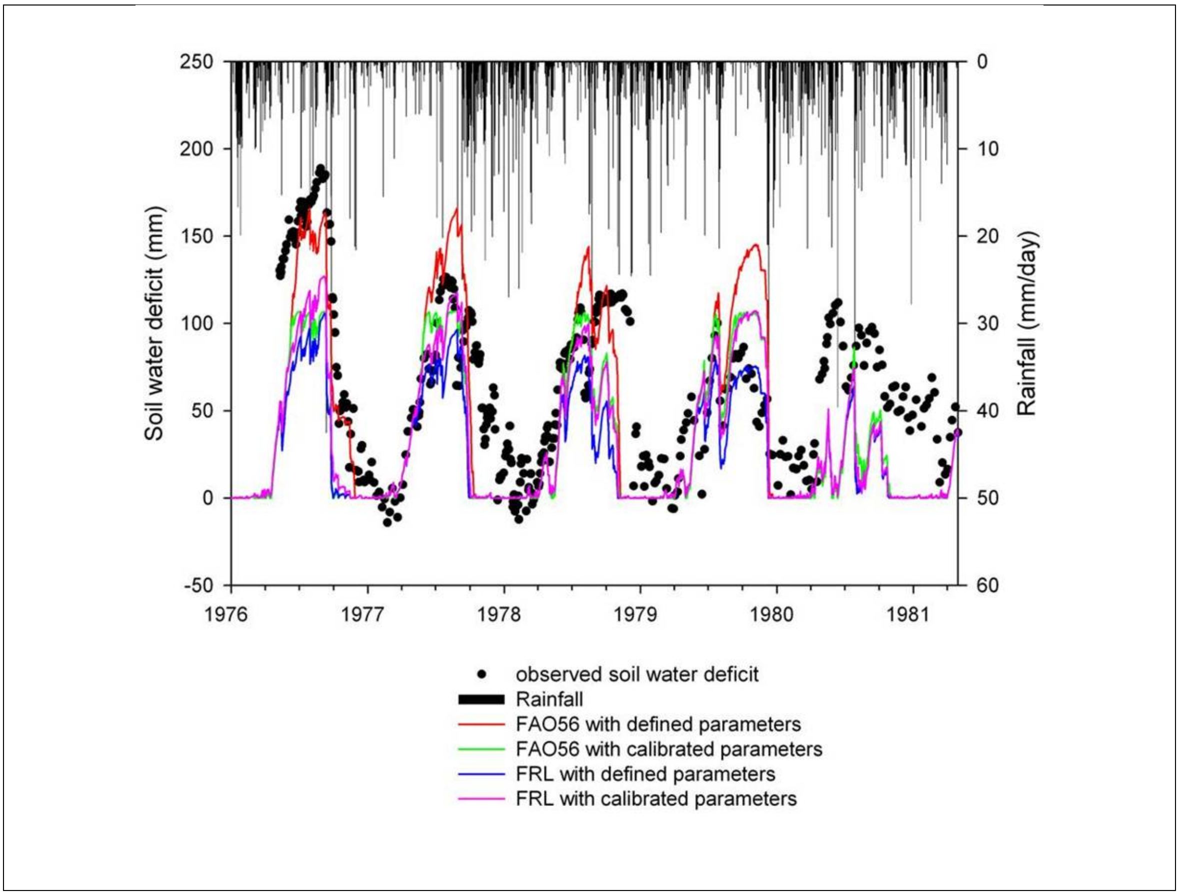

Figure 4.3 Simulated and observed soil water deficits at Bridgets Farm

The RMSEs for the four combinations of soil water models and parameters for the data at Fleam Dyke, Table 4.3, are very similar, although the lowest is for the FRL soil water model with the calibrated parameters and the largest is for the same model with the defined parameters. The time series, Figure 4,4, again show that the FAO56 soil water model with defined parameters performs well in predicting the soil water deficits during dry summers and that there is little to choose between either soil water model when the calibrated parameters are used. Thus the results with these data are very similar to those with the data from Bridgets Farm.

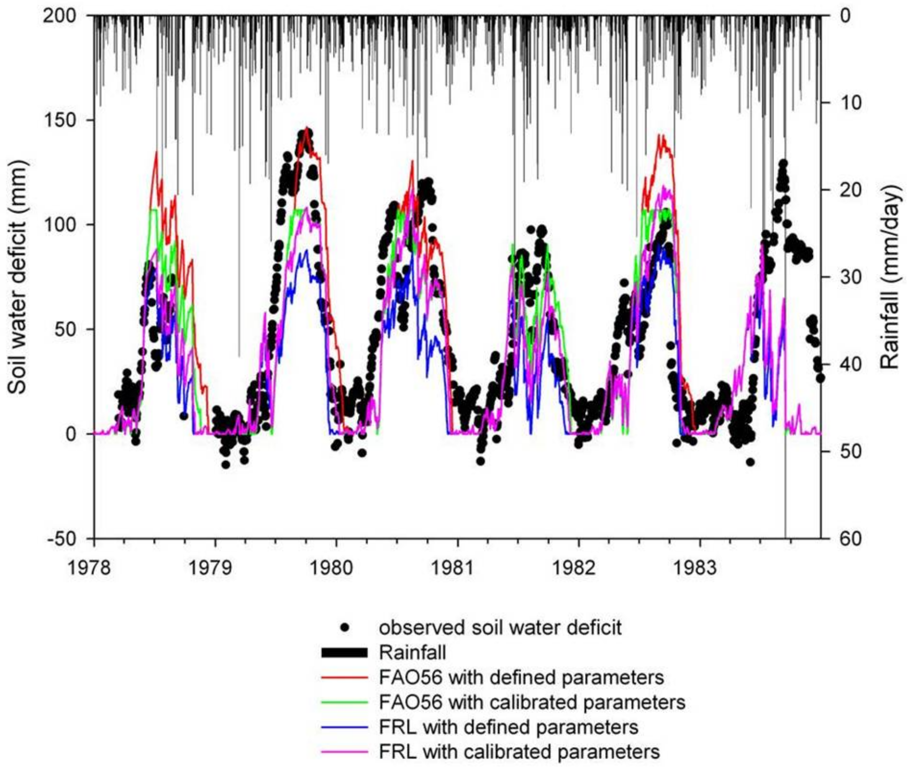

Figure 4.4 Simulated and observed soil water deficits at Fleam Dyke

The FRL soil water model gives a lower RMSE, Table 4.3, for the simulated soil water deficits against the measured values at Bicton. However, an examination of the time series, Figure 4.5, shows that neither model can be considered to do particularly well. In part this is because the value for the available water content, 109 mm, is lower than is appropriate – demonstrated by the range of the measured soil water contents being around 140 mm. In general, the FAO56 soil water model tends to simulate the soil water deficits better than the FRL model during dry summers, whilst the converse is true during wet summers. The timing of development and elimination of soil water deficits is fairly similar although the FAO56 soil water model consistently gives a later date each year, implying slightly less recharge.

The RMSE for the soil water deficits simulated by both soil water models at Bacon Hall are exceptionally large, Table 4.3. As is the case with the data from Bicton, this is dominantly because the value for the available soil water being too low, as shown by the time series, Figure 4.6. A value of at least 150 mm would appear to be more appropriate for this site. In addition, significant negative soil water contents are observed during most winters. There are known to be peizometric surfaces at around 3.8 and 1.5 m depth but an examination of the neutron probe measurements suggest that saturated conditions are observed at 0.8 m during most winters, suggesting that either there is an additional peizometric surface or that the water table associated with the shallower one can come up to a depth of less than 0.8 m. This also has an implication for the evaporation from the site as it is possible that soil water stress may not occur in all summers, e.g. during 1987, although it will be present during particularly dry summers, e.g. 1990. Thus the results for the data from this site should be used with caution.

In summary, the analysis of the model simulations of soil water deficits for the long term sites does not show any clear advantage of one model over the other. It would appear that the issue is dominantly of how appropriate the parameter values are to conditions at the measurement site.

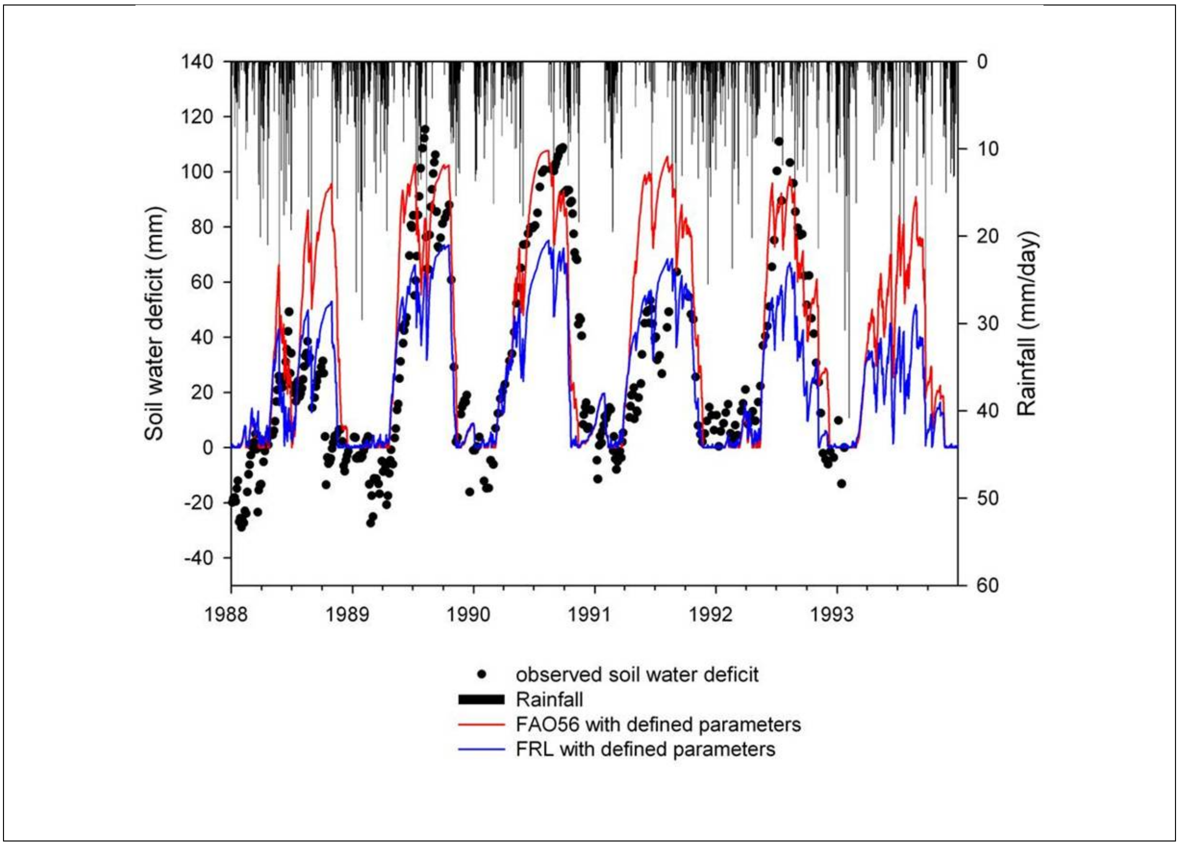

Figure 4.5 Simulated and observed soil water deficits at Bicton

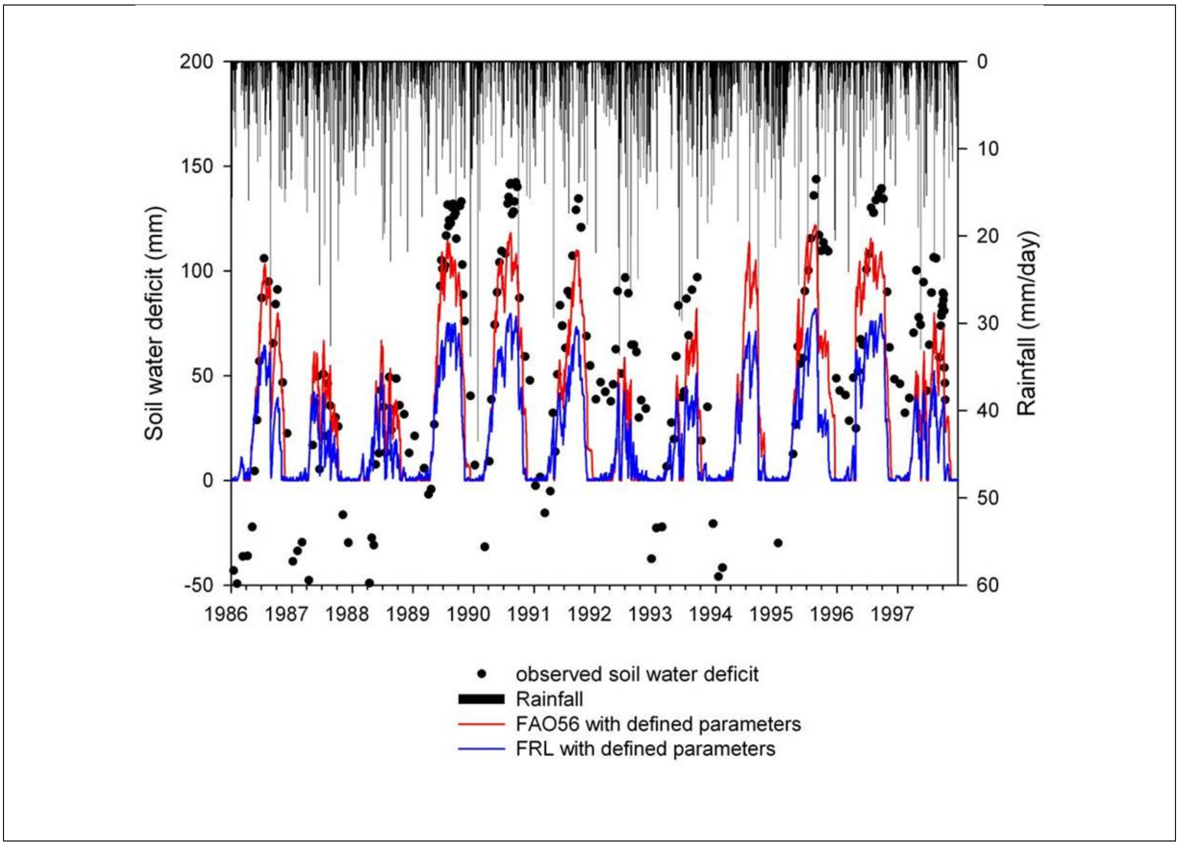

Figure 4.6 Simulated and observed soil water deficits at Bacon Hall

4.3 Model parameter sensitivity

The sensitivity of the soil water models to parameter values has been investigated using the data from the Sheepdrove Farm site with a Monte Carlo approach. 50,000 parameter sets were generated at random, with the range for each parameter constrained to lie within a range that was physically possible. Two parameters are required for the FAO56 soil water model whilst three are needed for the FRL model. A similar exercise was carried out for the data from Highfield Farm but the results are virtually indistinguishable and so have not been included.

The results for the FAO56 soil water model are shown in Figure 4.7. It is clear that there are many combinations of the two parameters which will achieve essentially the same RMSE. However, the model is more sensitive to the available soil water than the critical soil water content. As the available soil water content increases, the minimum RMSE reduces rapidly but then the change slows down and there is a broad range of values over which the minimum RMSE changes relatively little. In comparison there is relatively little change in the minimum RMSE as the critical soil water content changes. This is because it is the available soil water content that controls the size of the soil water deficits over much of the range with the critical soil water content modifying the soil water deficit, through reducing the evaporation rate as the soil water deficit increases, at greater soil water deficits.

The FRL soil water model shows a similar pattern, albeit that the introduction of a third parameter results in an even clearer pattern of many parameter sets producing the same outcome. Again there is a minimum available water content, below which the RMSE increase rapidly and above which there is relatively little change in the minimum RMSE. The second most sensitive parameter is the depth above which 65% of the roots occur, z_{65}, for which there is clearly a value which produces the lowest RMSE. In comparison, the model is relatively insensitive to the critical soil water content.

The available soil water content as used by these models is dependant on two data sources, the first is the volumetric soil water content, which is a property of the soil, and the second is the rooting depth. When the absolute values that these parameters take is considered, then the rooting depth has the greatest effect. However, when the percentage uncertainty of the parameters is considered then the two are of equal important because they are multiplicative.

In summary, the available water content is the most critical parameter with both models and underestimating the value, compared to the optimum values is more likely to result in a significant increase in the RMSE than in overestimating it.

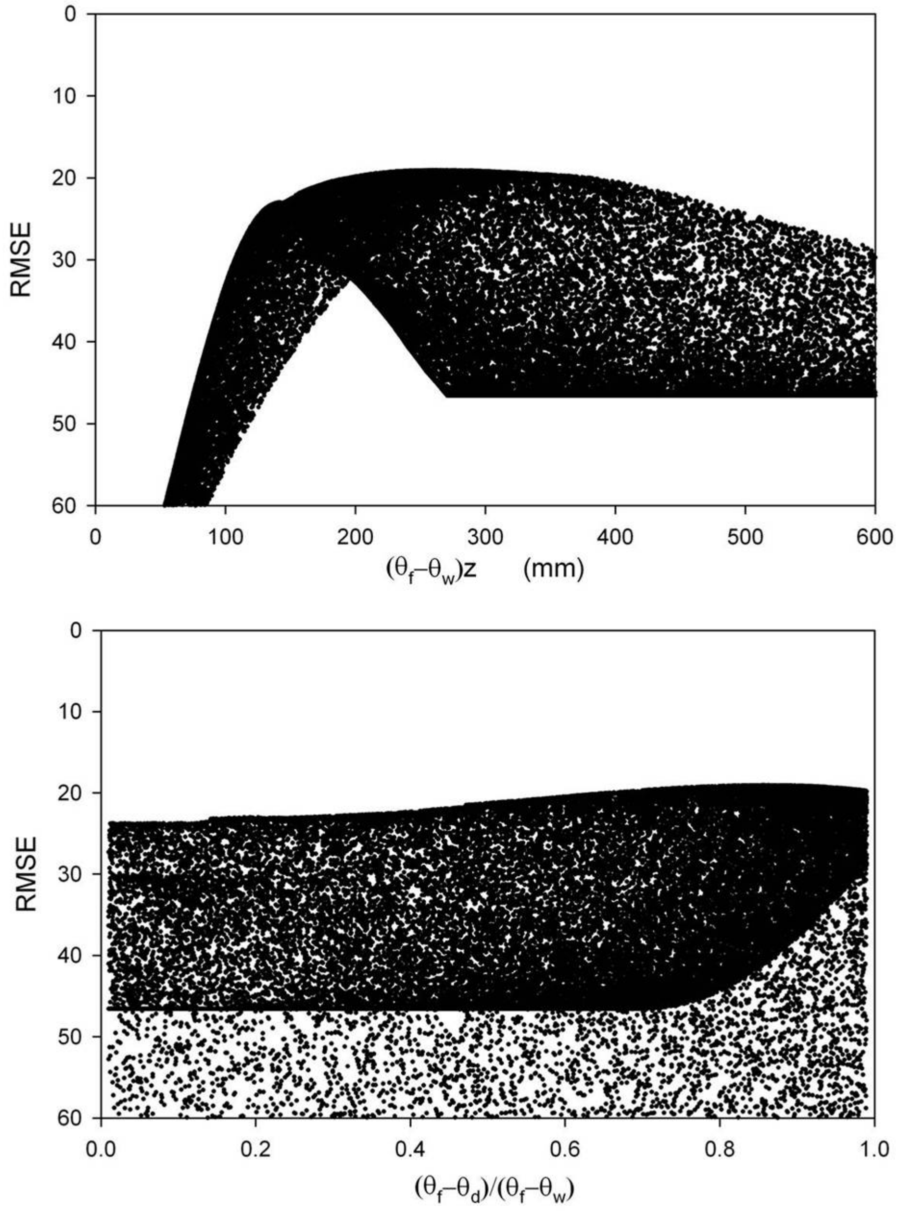

Figure 4.7 Parameter sensitivity for the FAO56 soil water model

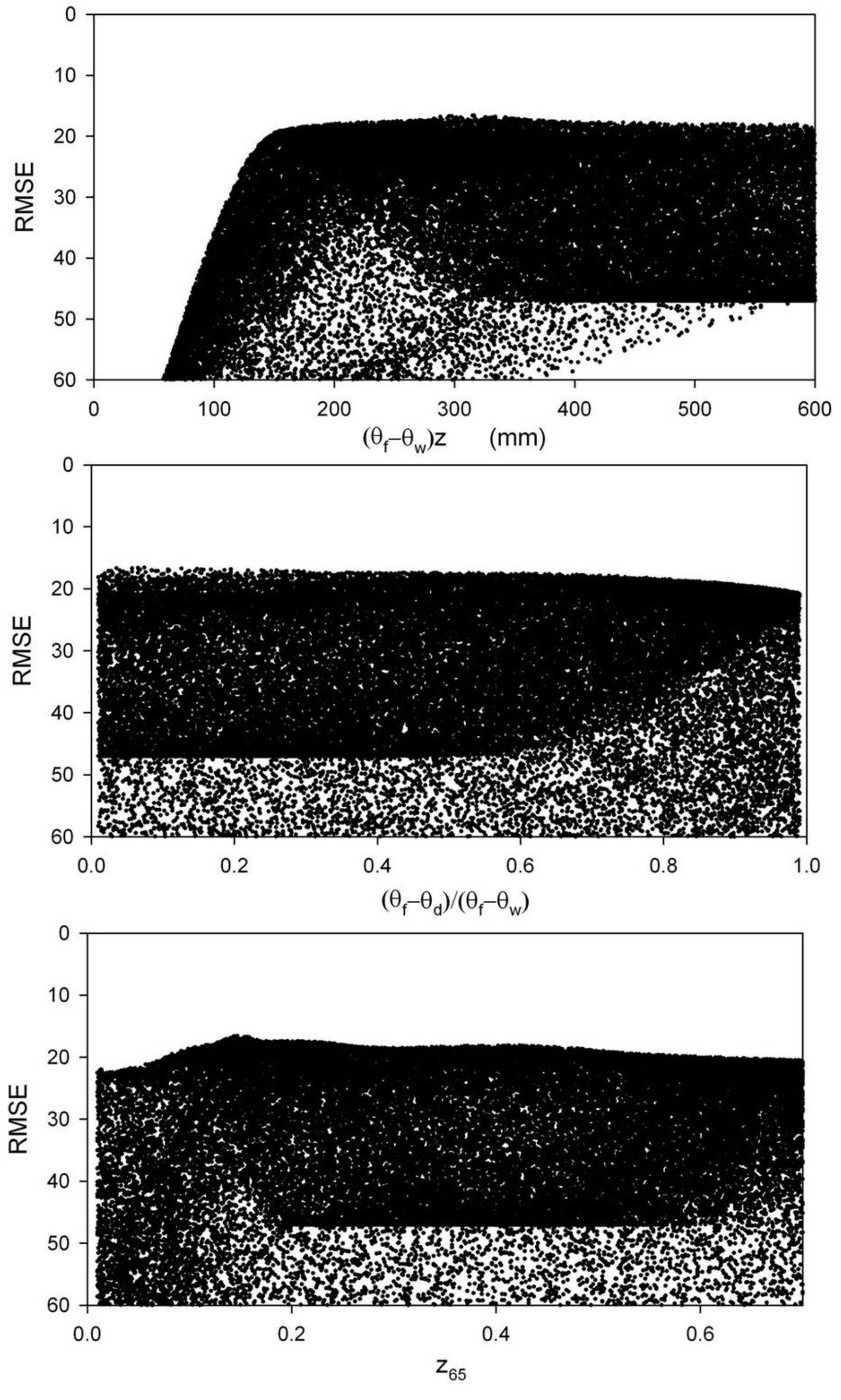

Figure 4.8 Parameter sensitivity for the FRL soil water model

4.4 The MOSES soil water model

It is not possible to make a direct comparison between the MOSES soil water model and the FAO56 and FRL soil water models because the parameters used by the former are different to those used by the other two. Nevertheless it is useful to make a limited comparison because of the very different model structure of the MOSES soil water model which is representative of those that simulate unsaturated flow.

A full description of the MOSES soil water model is given in Section 7.3. It is based on a finite difference approximation to the Richards' equation (Richards, 1931) for unsaturated flow through porous media, The soil is divided into four vertical layers with thicknesses of 0.1, 0.25, 0.65 and 2 m. The same soil hydraulic parameter values are used for each layer in the operational implementation of the soil water model. The van Genuchten *et al* (1991) model of the forms for the hydraulic conductivity and the soil water suction as a function of the soil water content is used. The distribution of roots is based on an exponential decrease with depth down to a defined maximum rooting depth.

Finch and Haria (2006) have carried out a study of the MOSES soil water model against the measurements at Sheepdrove Farm. As part of the study they calibrated the soil water model parameters against the measured soil water contents whilst driving the model with the measured evaporation and rainfall at the site. Although this approach is similar to that used in this study, there were important differences:

- An hourly time step was used for the model runs;
- The calibration was based on comparing the simulated with the observed soil water contents whilst considering each of the model layers as separate conditions;
- The calibration was for all four layers, i.e. down to a depth of 3m;
- the diagnostic variable was the soil water content (c.f. the soil water deficit used in this study).

The latter condition is because the concept of a field capacity is not in the formulation of the soil water model. A value for a "field capacity" can be obtained by running the soil water model, initialised at saturation, with no driving data for a time period of about 3 months, i.e. allowing the soil water model to "drain" to a static condition.

Nevertheless, it is possible to make a comparison with this study by:

- Calculating the mean of 24 hourly values to produce average daily values of the soil water content;
- Summing the soil water contents of the topmost three layers to give a total soil water content for a depth down to 1 m;
- Calculating the soil water deficit using the same value for the field capacity used in this study.

It is emphasised again that care must be taken in comparing the results from the two studies because the MOSES soil water model was being used to simulate the soil water contents down to 3 m whilst this study has only considered 1 m.

The RMSE obtained was 13.9 mm, which is significantly lower than those obtained from the FAO56 and FRL soil water models, Table 4.1. It is likely that a significant proportion of this reduced RMSE is due to the MOSES soil water model being able to simulate the changes in soil water content during the winter months much more convincingly, see Figure 4.9.

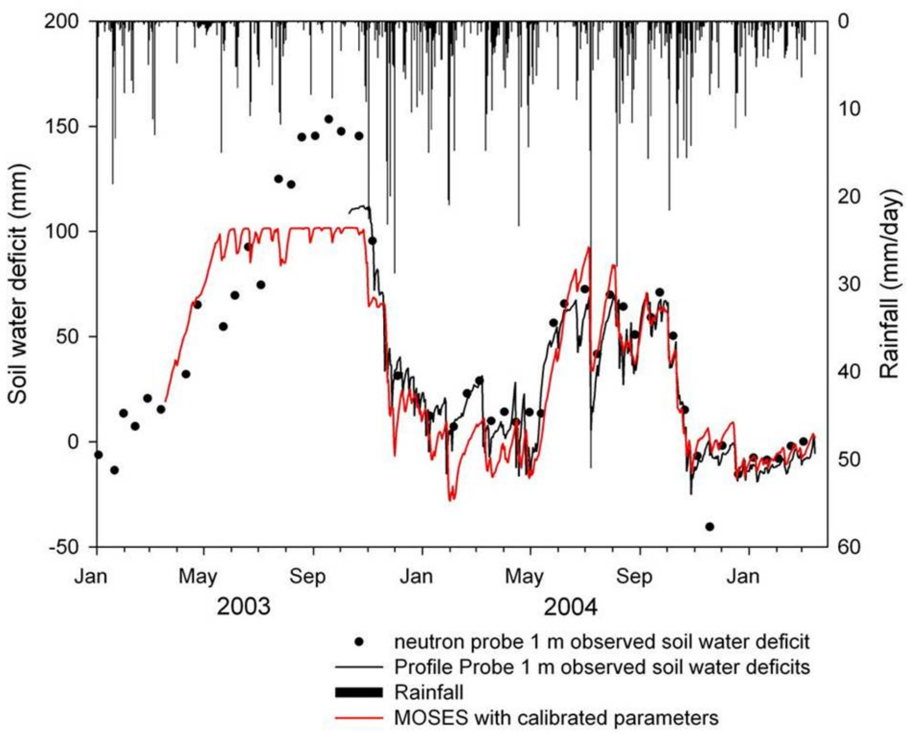

Figure 4.9 MOSES soil water model simulated and observed soil water deficits at Sheepdrove Farm

The simulated values during the summer months are comparable to those obtained with the FAO56 and FRL soil water models, Figure 4.1. Although the MOSES soil water model appears not to simulate the soil water deficits during the summer of 2003 particularly well this is because only the top 1 m of the soil profile is considered here. Significant depletion of the soil water is simulated in the bottom model layer, i.e. between 1 and 3 m depth, with a result that the model does a good job of simulating the soil water contents through the full 3 m soil profile but, as a consequence of using the same soil hydraulic parameter values in each layer, it tends to over estimate the soil water contents near the surface and under estimate them at depth.

In conclusion, the MOSES soil water model performs significantly better, than the FAO56 and FRL soil water models, at simulating the observed soil water contents throughout the year, mainly because the model is a more physically correct representation of the soil water processes. This improvement is achieved at the cost of significant increases in model complexity and computational time.

5 Discussion

This study has been concerned with data from sites that can be considered, especially at the scale of the soil water measurements, as points. Thus it is unable to make any unambiguous comment about how the heterogeneity in the landscape may impact estimates of recharge. This particularly applies when considering soil water model parameters derived from NSRI's data. The latter are the "average" values pertaining to a particular soil series and so are not necessarily those appropriate to a particular site.

This study has shown that at two of the sites, Highfield Farm and Bacon Hall, the soil water down to a depth of 1m is probably influenced by water tables and so do not consistently conform to the assumption made in the soil water models that drainage of the soils is not inhibited by groundwater. Thus the results from these sites must be interpreted with a degree of caution.

5.1 Model structure

Both the FAO56 and FRL soil water models use the capacity approach, i.e. that drainage only occurs at soil water contents above a threshold that is a property (the field capacity) of the soil and assume that drainage takes place with a single time step (one day was used in this study). Similarly, evaporation from the soil and transpiration take place at a rate (the potential rate) determined by the driving variables until the soil water content is reduced to a critical soil water content. At soil water contents lower than this threshold the evaporation rate is reduced as a linear function until the soil water content at wilting point is reached when all evaporation ceases. The difference between the two soil water models is that, in the FAO56 model, the soil (defined as the depth to the maximum rooting depth of the vegetation) is a single, homogeneous "layer", whilst the FRL model considers the soil to consist of four vertical layers of equal thickness with, in the case of this study, the same hydraulic properties. This requires an additional parameter that defines the fraction of the total roots in each layer.

By driving the soil water models with the measured evaporation and calibrating the soil water model parameters, Section 4.1, this study has shown that the model structure of the FRL soil water model results in lower uncertainties than that of the FAO56 soil water model. It is not simply because of the addition of an additional parameter but is also because the model structure allows the model to be more "responsive" to rainfall and evaporation. This is particularly noticeable in the models' ability to simulate high evaporation rates after rainfall in the presence of soil water deficits (for example see the simulated soil water contents for Sheepdrove Farm in September and October of 2003, Figure 4.1). It also shows in a more progressive reduction in evaporation rates as a soil water deficit develops. This is potentially important in allowing recharge to occur in the late spring if a dry early spring is followed by a period of heavy rainfall. The differences in the model structures are less important, when simulating the soil water contents in the autumn, because both models tend to simulate similar "maximum" soil water deficits in the late summer/early autumn as it is the model parameter value (the available soil water content) that determines this.

Because of the use of the capacity approach, neither model is particularly good at simulating slow drainage, i.e. over periods of several days or longer. This is most obvious during the winter periods when the values of soil water content simulated by the soil water models tend to show very little variability compared to the measurements. This is not a problem provided that the estimates of soil drainage (and thus recharge) are required for time steps longer than the time scale of the soil water drainage. In the case of many groundwater applications the time period is between one week and one month and so this condition is fulfilled in the case of free draining soils but may not be so in slow draining soils, such as those with a high clay content. It is not the case with chalk soils and this will be discussed further in Section 5.3.

Neither soil water model considers the possibility of water flowing by bypassing the soil matrix. Of the sites considered, this is only likely to occur for those with chalk soils. The work in this study has not considered this element of soil water because the measurements do not directly or indirectly allow this condition to be recognised. The issue will be further discussed in Section 5.3 but it should be noted that Finch (1998), in analysing the sensitivity of estimates of recharge to the land surface description, concluded that the amount of effective precipitation bypassing the soil matrix was not an important parameter.

5.2 Model parameters

The uncertainties in the simulated soil water contents increase when using model parameters derived from the NSRI's data, compared to those simulated using calibrated parameter values (see Tables 4.2 and 4.3), as would be expected. However, in terms of simulating the timing of the beginning and end of soil water deficits, and thus the period of recharge, the differences are less marked, although the FAO56 soil water model, parameterised with values from the NSRI's data, consistently simulates a later end and thus a lower annual recharge.

The calibrated values of the available soil water content for the FRL soil water model are higher than those for the FAO56 at both LOCAR sites (see Table 4.1), reflecting the differences in the model structures. Given that, operationally, the soil water model will use parameter values derived from the NSRI's data, the question arises as to which model structure is more appropriate to these parameter values? In theory, it should be the FRL soil water model because its model structure reflects the observation of a reduction in soil water deficits with depth correlating with a similar reduction in root density. But, is this confirmed by this study? An examination of the RMSEs for the two models at all the sites (Tables 4.2 and 4.3) suggests that there is little evidence for this, which leads to the conclusion that it is the parameter values appropriate to a given site that are more important than the model structure.

In terms of the parameter sensitivity, the conclusions are the same for both soil water models: it is the available soil water that is dominant, although there are a wide range of parameter sets that can result in similar values of the RMSE. The available soil water is derived from two other parameters: the fractional available water content (a property of the soil) and the rooting depth of the vegetation, both of which show variability within given types and may be correlated, e.g. when the soil condition limits the developments of roots. Unfortunately there is very little information in the literature about how much variability there is in these two parameters so it is not possible to make any useful statements about the uncertainties associated with using an "average" value when simulating the soil water contents at the landscape scale. The use, in this study, of fractional available water contents derived from the NSRI's data for specific sites suggests that there is significant variation around the "average" value, but whether this is important at the scale of model grid cells is unclear.

5.3 Chalk soils

Simulating the soil water content of chalk soils is particularly challenging to hydrologist because of the small diameter of the pore throats, resulting in suctions increasing rapidly for a comparatively small reduction in the soil water content, and due to the presence of fractures, resulting in a dual permeability media. The FAO56 and FRL soil water models have a very limited ability to reproduce these features, because the processes are not explicitly represented, and so this study can not deal with issues such as bypass flow or slow drainage. However, research has been going on into the hydraulic properties of the chalk, integrating measurements and modelling, and the results are just beginning to appear in the literature. Mathias *et al*. (2005) and Mathias *et al*. (2006) report the results of numerical modelling, the latter using a transient dual-permeability model of flow and solute transport (which has 18 parameters). Although the model simulations are not explicitly compared with observations, the observations are used qualitatively to constrain the parameter values. Thus, these studies explored the range of parameter values that allow the observed features of flow and transport in the soil and unsaturated zones of the chalk to be simulated. The main observed phenomena are: a fast water table response, an absence of surface runoff, slow solute migration and very littler solute dispersion. The results showed that infiltration has to be appreciably attenuated so that enough flow occurs through the matrix in order to reproduce the observed solute spreading. This attenuation was attributed to the presence of soil and gravely chalk above the solid chalk, i.e. that the zone from the surface down to about 0.8 m is extremely important in modifying the flow and transport. However, the model was still able to reproduce a rapid (3 days) response in the water table at a depth of 10 m. It was concluded that fracture flow in the unsaturated zone was episodic and infrequent, representing between 17% and 30% of the annual recharge, which is in agreement with observations, e.g. Jones and Cooper (1998).

Ireson *et al*. (2006) analysed measurements of soil water content and matric suction, made on the Berkshire Downs as part of the LOCAR programme, and showed that the results of Mathias et al. (2006) were compatible with these. In particular that the top 1 m of the profile acts to attenuate the changes at the surface. They also concluded that the measurements were consistent with a displacement mechanism whereby flow occurs dominantly through the matrix. Thus, changes in the soil water contents in the near surface cause the rapid propagation of matric suction down to the water table; increasing or decreasing the downward hydraulic head gradient at the water table and hence increasing or decreasing the rate of recharge. A consequence is that recharge is likely to occur continually throughout the year, albeit at varying rates; which is supports the conclusion of Lewis *et al*. (1993) that a significant part of the storage in the chalk is in the unsaturated zone. The measurements of matric suction show that the occasions on which the suctions were low enough through the whole soil profile for fracture flow to occur were very infrequent. This was also confirmed by Finch and Haria (2006) using a modified form of the MOSES soil water model to simulate observations.

Subsequently, Ireson (pers. comm.) has extended his work by including additional observations and developing a dual permeability numerical model based on Richards' equations. This has served to confirm the previous analysis of measurements and has also served to emphasise the crucial role of the top 1 m of the profile in modifying the infiltration. It also demonstrates that the capacity approach, as used in the FAO56 and FRL soil water models, is not appropriate to an explicit representation of the full profile of chalk soils, within which soil water deficits occur, although it might be possible to use them for the upper part, less than 0.8 m, of the profile.

It should be noted that the chalk should not be regarded as having the same hydraulic properties through out its outcrop e.g. whereas Jones and Cooper (1998) concluded that fracture flow did occur at a site in Cambridgeshire, the results from the LOCAR programme suggest that its presence cannot be recognised in the Berkshire Downs.

6 Conclusions

- The model structure of the FAO56 soil water model results in greater uncertainties in simulated soil water deficits than are achieved with the FRL soil water model;
- The model structure of the FRL soil water model allows it to simulate the development of soil water deficits more successfully than the FAO 56 sol water model;
- Neither the FAO56 not the FRL soil water models simulate slow drainage of the soils, a feature particularly apparent during the winter months;
- Both soil water models are most sensitive to the value of the available soil water parameter and relatively insensitive to the other parameter values
- Both soil water models can produce simulations of soil water deficit with relatively similar uncertainties with a range of parameter sets;
- Uncertainties due to the value of the available water content are greater than those due to the differences in the soil water model structures;
- There is very little information available about the variability in the fractional available soil water of a soil series or of the rooting depth of a vegetation type;
- The use of a soil water model based on the Richards' equations of unsaturated flow, such as used in MOSES, provides a better description of drainage than those based on the capacity approach, but this is at the cost of a significant increase in computational time and the number of model parameters;
- Recent research has demonstrated the importance of matrix flow in the unsaturated chalk and constrained the range of flow through fissures;
- Recent research has demonstrated the importance of the upper part of the profile, ca 0.8 m, of chalk soils in attenuating the inputs.

7 Annexe 1 – Soil water models

7.1 FAO56

The soil water model described in the FAO Irrigation and Drainage Paper 56 (Allen *et al*. 1998) is based on the capacity approach and use a simple water balance conceiving of the soil water storage as a single store. The soil water content for the i^{th} time step is calculates as:

$$\theta_i z = \theta_{i-1} z + W_{0,i} - E_{a,i}$$

Where:

$E_{a,i}$	actual evaporation, i.e. the water uptake by roots
$W_{0,i}$	the effective precipitation, i.e. precipitation + irrigation - interception
z	thickness of the soil
θ_j	volumetric soil water content

If the volumetric water content exceeds the water content at field capacity then it is set to the latter and the excess is allocated to infiltration, *W*, i.e.:

$$W_i = (\theta_i - \theta_f) z$$

This implies an assumption that the soils drain down to the water content at field capacity within a period of less than one day.

The actual evaporation is calculated using a stress factor, *S*. Initially, this factor is set to 1 so that the evaporation continues at potential, until a critical volumetric water content is reached. Below this water content the stress factor decrease linearly from a value of 1 to that of 0 at the volumetric water content at wilting point , i.e.:

$$S_i = \frac{\theta_i - \theta_w}{\theta_d - \theta_w} \qquad \theta_w < \theta_i < \theta_d$$

$$S_i = 0 \qquad \theta_i \leq \theta_w$$

$$S_i = 1 \qquad \theta_i \geq \theta_d$$

where

$E_{p,i}$	potential evaporation for the land cover
θ_d	citical volumetric soil water content, i.e. below which evaporation is reduced below potential
θ_f	volumetric soil watercontent at field capacity
θ_w	volumetric soil water content at wilting point

Using the terminology of Allen *et al*. (1998), p_5, the average fraction of Total Available Soil Water (TAW) that can be depleted from the root zone before water stress occurs, when the potential evaporation rate for the land cover is approximately 5 mm/day, is:

$$p_5 = \frac{\theta_f - \theta_w}{\theta_f - \theta_d}$$

The factor, p, is also a function of the potential evaporation rate:

$$p = p_5 + 0.04(5 - E_p)$$

7.2 FRL

The Four Root Layer (FRL) soil water model is also based on a capacity approach (Ragab *et al*., 1997) . If the inflow, i.e. the effective precipitation, to the first layer exceeds field capacity then the excess water drains down to the second layer and so on for each of the layers. Please note, in this and the following section, the time step subscript has been omitted in the interests of clarity.

The flow of water, W_j, downwards into each layer of the soil model is calculated as

$$F_j = W_0 \qquad j = 1$$

$$F_j = F_{j-1} - (\theta_{f,j-1} - \theta_{j-1})\Delta z_{j-1} \qquad j > 1$$

$$F_j = 0 \qquad F_{j-1} < (\theta_{f,j-1} - \theta_{j-1})\Delta z_{j-1}$$

where:

W_0	the effective precipitation (mm), i.e. precipitation + irrigation - interception
Δz_j	thickness of the soil layer
θ_j	layer volumetric soil water content
$\theta_{f,j}$	layer volumetric soil water content at field capacity
$\theta_{w,j}$	layer volumetric soil water content at wilting point

This implies an assumption that the soils drain down to the water content at field capacity within a period of less than one day.

The infiltration, W_4, ,i.e. the flow downwards from the deepest (fourth) layer, is calculated as:

$$W_4 = F_4 - (\theta_{f,4} - \theta_4)\Delta z_4 \qquad F_4 > (\theta_{f,4} - \theta_4)\Delta z_4$$

$$W_4 = 0 \qquad F_4 \le (\theta_{f,4} - \theta_4)\Delta z_4$$

As in the FAO56 model, the maximum available water for plant water uptake is defined as the difference between the soil water content at field capacity and wilting point. Plant roots take up water at the maximum rate, i.e. potential evaporation, until a critical soil water content is reached. The rate of water uptake then decreases linearly, from its maximum, to zero when the soil water content falls below the wilting point. The contribution of each of the soil layers to the total root water uptake, and hence the actual evaporation, depends on the proportion of roots in the layer. The distribution of active roots in a normal soil is approximately triangular in shape, the greater concentration being near the surface (Hansen *et al*., 1979) and thus the proportion of roots, per unit thickness, will be greater in the top layer. The function used to describe this in the model is that of Gerwitz and Page (1975)

$$V_z = 1 - e^{-z/z_{65}}$$

where:

V_j	fractional proportion of roots down to depth z
Z_{65}	the depth, above which 65 % of the roots occur

The stress factor, applied to the potential evaporation, is used to calculate the root water uptake and, for the j[th] layer, is calculated as:

$$S_j = \frac{\theta_j - \theta_{w,j}}{\theta_{d,j} - \theta_{w,j}} \qquad \theta_{w,j} < \theta_j < \theta_{d,j}$$

$$S_j = 0 \qquad \theta_j \le \theta_{w,j}$$

$$S_j = 1 \qquad \theta_j \ge \theta_{d,j}$$

where:

S_j	stress factor used to reduced water uptake by roots
$\theta_{d,,j}$	critical volumetric soil water content, i.e. below which evaporation is reduced below potential

The actual root water uptake is then calculated as

$$E_{a,j} = E_p S_j V_j$$

where:

$E_{a,j}$	actual water uptake by roots
E_p	potential evaporation for the land cover
V_j	fractional proportion of roots in the layer

7.3 MOSES

The following is taken from Essery *et al.* (2001). The soil water component of the Met. Office Surface Energy Scheme (MOSES) is based on a finite difference approximation to the Richards' equation (Richards, 1931) of flow in unsaturated porous media, with the vertical discretization into four layers. Thus the model is based on the explicit representation of the movement of water between layers. The prognostic variables of the model are the total soil water content, *M*, within each layer:

$$M = \Delta z \theta_s \left(\rho_w S_u + \rho_i S_f \right)$$

where Δz is the thickness of the layer, ρ_i and ρ_w are the densities of ice and water respectively, θ_s is the volumetric soil water content at saturation. The unfrozen and frozen volumetric soil water contents, θ_u and θ_f respectively, are expressed in non-dimensional form as $S_u=\theta_u/\theta_s$ and $S_f=\theta_f/\theta_s$.

In the van Genuchten (1980) formulation of soil hydraulics soil water contents are expressed as excesses over the residual volumetric soil water content (i.e. the water that is fixed in the soil), θ_r, so:

$$\Theta_u = \frac{\theta_u - \theta_r}{\theta_s - \theta_r}$$

$$\Theta_f = \frac{\theta_f - \theta_r}{\theta_s - \theta_r}$$

In practice the differences between S_u and Θ_u and between S_f and Θ_f are often ignored in the expression for M.

The total soil water content within the n^{th} soil layer is incremented by the diffusive water flux flowing in from the layer above, W_{n-1}, the diffusive flux flowing out to the layer below, W_n, and the evapotranspiration extracted directly from the layer by plant roots and soil evaporation, E_n:

$$\frac{dM_n}{dt} = W_{n-1} - W_n - E_n$$

E_n is calculated from the total evapotranspiration, E_t, based on the profiles of soil water and root density, $E_n = e_n E_t$. The root density is calculated assuming an exponential decrease with depth. Thus the fraction of roots in the j^{th} layer, r_j is given by

$$r_j = \frac{e^{-ez_{j-1}/d_r} - e^{-2z_k/d_r}}{1 - e^{-2z_t/d_r}}$$

where d_r is the rooting depth of the vegetation type, z_{j-1} is the depth to the top of the layer, z_j is the depth to the bottom of the layer and z_t is the total soil depth in the model.

The water fluxes are given by the Darcy equation:

$$W = K \left(\frac{\partial \Psi}{\partial z} + 1 \right)$$

where K is the hydraulic conductivity and Ψ is the soil water suction. To close the model it is necessary to assume forms for the hydraulic conductivity and the soil water suction as a function of the soil water concentration. The dependencies suggested by van Genuchten (1980), have been included:

$$\Psi = \frac{\left(\Theta_u^{-1/m} - 1\right)^{1/N}}{\alpha}$$

$$K = K_s \Theta_u^{1/2} \left\{1 - \left(1 - \Theta_u^{1/m}\right)^m\right\}^2 = K_s \frac{\left\{1 - (\alpha\Psi)^{N-1} \left\{1 + (\alpha\Psi)^N\right\}^{-m}\right\}^2}{\left\{1 + (\alpha\Psi)^N\right\}^{m/2}}$$

$$m = 1 - \frac{1}{N}$$

where the saturated hydraulic conductivity, $K_{s,}$ and α and N are empirical soil dependent constants. The interpretation of the van Genuchten relationships in terms of unfrozen rather than total soil water is consistent with the observation that the freezing of soil water reduces hydraulic conductivity and produces a large suction by reducing the unfrozen water content (Williams and Smith (1989).

The top boundary condition for the soil hydrology module is given by:

$$W_0 = \sum_j \nu_j \left(T_{Fj} + S_{mj} - Y_j\right)$$

The default lower boundary condition corresponds to “free drainage":

$$W_n = K_n$$

where W_n is the drainage from the lowest deepest soil layer and K_n is the hydraulic conductivity of this layer.

MOSES includes an implicit scheme which remains numerically stable and accurate at relatively long timesteps and high vertical resolution. The prognostic equation is:

$$\frac{dM_n}{dt} = W_{n-1} - W_n - E_n$$

The soil water fluxes, W, are a function of the prognostic variables M_n. In the explicit MOSES the fluxes are calculated using a forward timestep weighting, , such that:

$$W_n = W_n^t + \gamma \frac{\partial W_n}{\partial M_n} \Delta M_n + \gamma \frac{\partial W_n}{\partial M_{n+1}} \Delta M_{n+1}$$

where ΔY_n is the increment to Y_n during the timestep t to t+Δt. The above equation can be substituted into the prognostic equation to yield a series of n simultaneous equations for the n prognostic variables:

$$a_n \Delta M_{n-1} + b_n \Delta M_n + c_n \Delta M_{n+1} = d_n$$

where:

$$a_n = -\gamma\Delta t \frac{\partial W_{n-1}}{\partial M_{n-1}}$$

$$b_n = \Delta z - \gamma\Delta t \left[\frac{\partial W_{n-1}}{\partial W_n} - \frac{\partial W_n}{\partial M_n} \right]$$

$$c_n = -\gamma\Delta t \frac{\partial W_n}{\partial M_{n+1}}$$

$$d_n = \Delta t \left\{ W_{n-1}^t - W_{n-1}^t - s_n^t \right\}$$

The left-hand side of this equation represents the explicit update to the variable M_n. Note that no implicit correction is made to the sink term, E_n, since this would require an unwieldy implicit update to the entire coupled soil hydrology, soil thermodynamics and boundary layer system. By treating this term explicitly the updates to the soil temperatures and soil waters are decoupled, such that these variables can be incremented independently on each timestep. The equations represented above are a tridiagonal set which can be solved routinely by Gaussian elimination.

Supersaturation in a soil layer can occur by two separate means. The first is a numerical artefact arising from the use of a finite timestep during which a very large quantity of incident water (for example from a very intense rainstorm) can overfill the top soil layer. This occurs very infrequently in the implicit soil scheme of MOSES. Nevertheless, supersaturation can still occur when drainage from the base of a soil layer is impeded (either by frozen soil water or an assumed reduction of K_s with depth). Under these circumstances it may be necessary to return the soil water content in a layer to the saturation value. The excess water in a soil layer is instead removed by lateral flow which contributes to a larger fast runoff component. This assumption is consistent with the soil numerics (which should not lead to supersaturation as a numeric artefact), and results in much better water budgets for permafrost regions.

As currently implemented in the Met. Office's operational models, the thickness of the layers, from the surface downwards, are 0.1, 0.25, 0.65 and 2 m. The parameters are the same in each layer.

8 Annexe 2 - Measurements

8.1 Soil water

Two instruments for measuring soil water content have been used: neutron probes and profile probes.

The neutron probe has been in use for several decades and so there is a considerable body of knowledge about the measurements made. The methods described by Bell (1987) formed the basis of the methodology used. It is manually operated and, at the LOCAR sites measurements were taken at approximately fortnightly intervals at a sequence of depths down to 4.1 m beginning at a depth of 10 cm and then at intervals of 10 cm down to 60 cm, followed by intervals of 20 cm down to 200 cm and then at intervals of 30 cm. At the other sites, measurements were made at time intervals between monthly and daily and at depth intervals similar to those used in the LOCAR programme.

Whilst the neutron probe is a well established technique, the Profile Probe (manufacturer Delta-T, model PR1) is a relatively new instrument and measures the soil water content via the dielectric constant of the soil surrounding the probe. It has the advantage of being data logged so that high temporal resolution data can be acquired, in this case every 15 minutes. Measurements are at depths of 10, 20, 30, 40, 60 and 100 cm.

8.1.1 Calibration and data quality control

Profile Probe data

For the data from Sheepdrove Farm, Figure 8.1, it is possible to track events corresponding to rainfall from depth to depth in a consistent way and there is a seasonal trend which seems very reasonable, i.e. high water contents in winter and low in summer. There is a clear diurnal variation in the values at all measurement depths, which has an amplitude of about 1 mV, corresponding to a variation in volumetric water content of about 0.005. It occurs in the measurements from all depths, suggesting that it is the above ground electronics that are the source of this error. It is observed in the data from all sites. Test in the laboratory were unable to duplicate this fluctuation in response to air temperature and so its cause has not been identified although, subsequently other studies have confirmed its existence and suggested that it is the soil temperature that is the cause (Verhoef *et al*. 2006). However, these fluctuations are sufficiently small and of short time period in comparison to the changes of interest, resulting from evaporation and rainfall, that it was decided that they could be ignored.

There are a number of points which are significantly at variance from the general trend, do not correlate across depths and, when an increase in water content is implied, do not coincide with rainfall events. Thus these are likely to be errors. An automatic method was used to detect and eliminated single points significantly diverging from the general trend. The points had to conform to the following criteria:

- the data points preceding and following the point being checked both had to be higher or both had to be lower in value;

- the differences between the value of the point being checked and the values of the two adjacent points had to be the same to within 5%;
- the point being checked had to have a difference of at least 15 mV , i.e. 0.03 of full range voltage, from the adjacent points.

The detected data value was replaced by the average of the measurement preceding and that succeeding. This methodology removed the majority of 'suspicious' points but a few remained. On inspection, these were groups of two to four points and were eliminated manually.

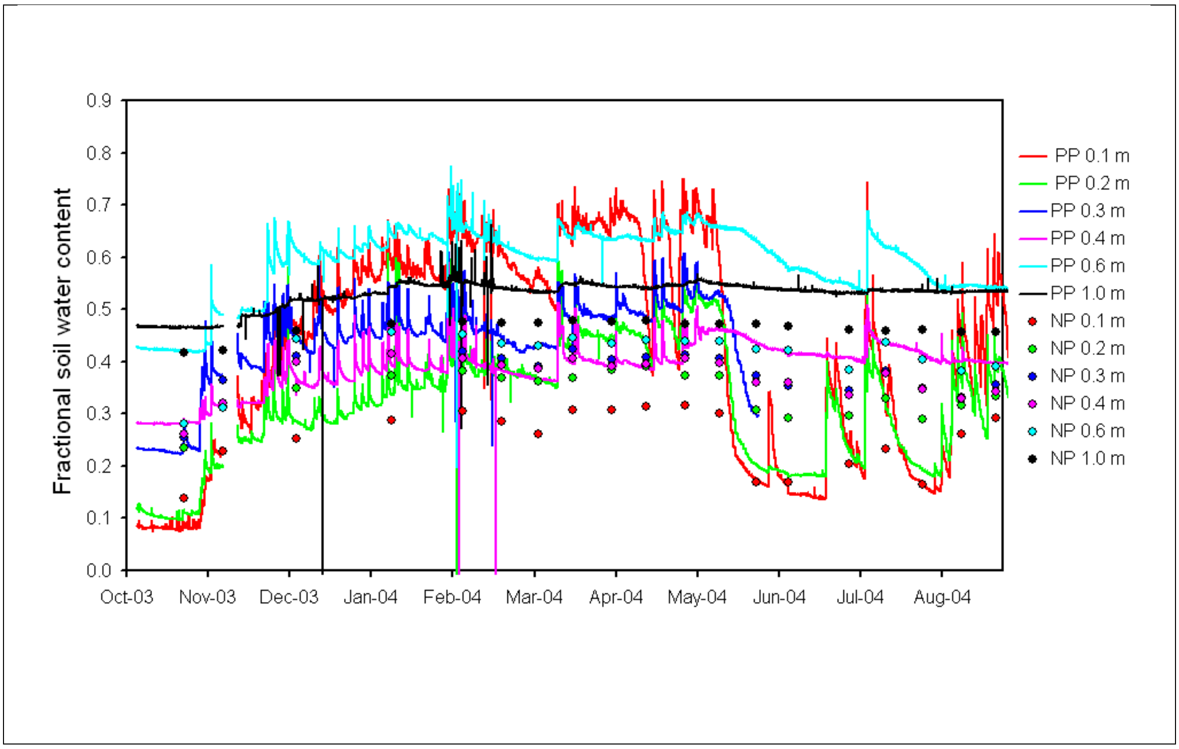

Figure 8.1 Comparison of soil water contents measured by neutron probe (NP) and a Profile Probe (PP) prior to quality control and calibration of the latter

When the profile probe measurements are compared with the corresponding neutron probe measurements, there is a consistent tendency for the profile probe measurements to be higher and for the maximum values to be higher than the range that would expect for this site. This suggests that the manufacturer's calibrations are not appropriate. The decision was made to calibrate the Profile Probe data against the neutron probe data, using two data points (the method recommended by the manufacturer). One of the data points selected was taken from a dry period, i.e. summer, whilst the other was taken from a wet period, i.e. winter. An additional criteria was that there should have been no rainfall in the preceding five days to ensure that the soil water contents were unlikely to be changing rapidly and thus reduce errors due to the timing of the readings from the two instruments. The calculated calibration coefficients were then applied to the Profile Probe data. The exception to this procedure was for the measurements at 10 cm for which measurements were made using a surface insertion capacitance probe (neutron probe measurements this near to the surface are unreliable due to the loss of neutrons into the air). These procedures resulted in significant differences to the data, Figure 8.2.

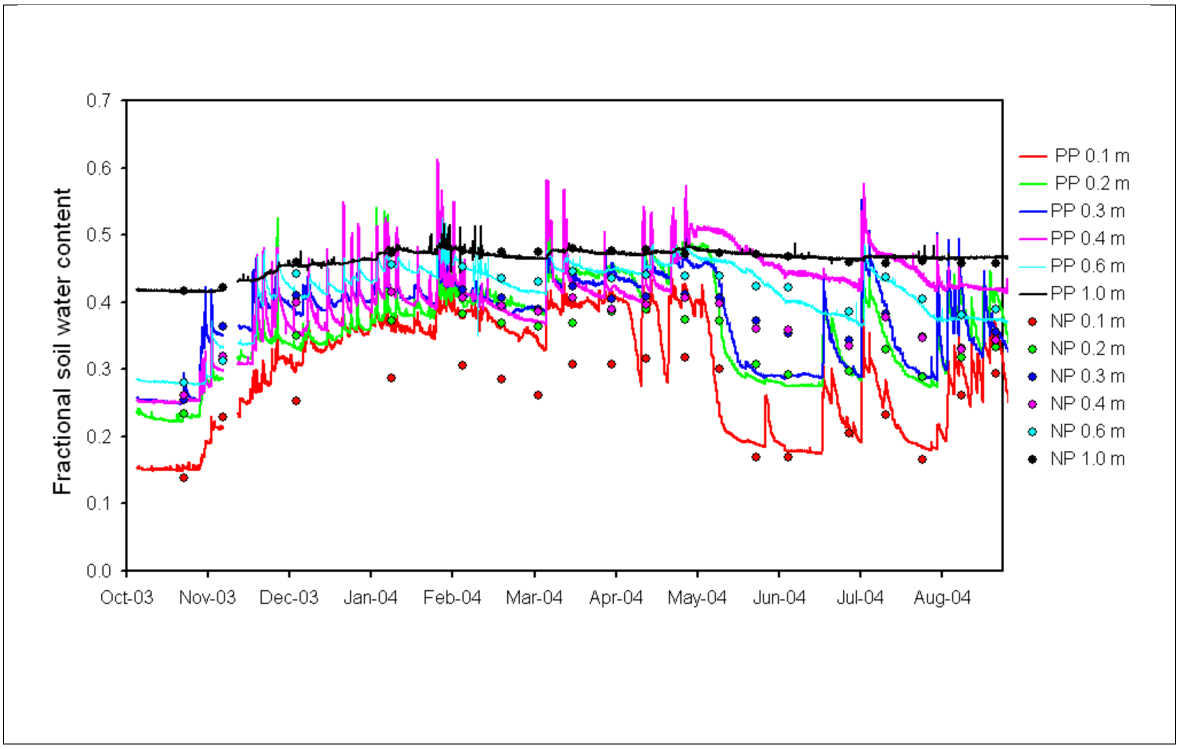

Figure 8.2 Comparison of soil water contents measured by neutron probe (NP) and a Profile Probe (PP) after quality control and calibration of the latter

Neutron probe data

The neutron probe data were quality controlled using a manual procedure. The data were graphed, both as time series and depth series, and points identified that don't match the general pattern. These were first checked against the original data sheet which allowed occasions when a written number has been incorrectly entered or that the readings had been written down in the wrong column (so attributing it to the wrong tube). These data were amended.

On some occasions it appears that there is a depth shift. This is usually very obvious if it is over quite a number of depths as the pattern associated with the different lithologies is translated with references to the readings taken on previous and subsequent dates, allowing the data to be edited to the correct depths.

If an individual reading does not seem to match the pattern then it is less certain that an error has occurred. It is usually fairly obvious if, for a given depth, there is a difference for one reading and then the readings return to about the previous level, plus the readings at the depths above and below do not show a similar change. This is attributed to an error in writing down the reading (e.g. transposing digits) so. It is often straight forward to work out what the reading should have been - but only gross errors can be identified, i.e. in the leftmost digit or if the middle digit is significantly wrong.

There are a few values that have been left in the dataset because it was not possible to be reasonably certain that there was an error.

8.2 Meteorology

Two sources of meteorological data have been used. The data from the two LOCAR sites, Sheepdrove Farm and Frilsham Meadow, are provided by automatic weather stations (AWS) logging measurements at hourly intervals. At the other sites the data are from daily, manual measurements.

8.2.1 Automatic weather station

The measurements made by the AWS, relevant to this study, are: soil heat flux, downward and upward shortwave radiation, downward and upward longwave radiation (and thus the net longwave radiation), relative humidity, wind speed and air temperature at heights of about 1.5 m above the ground. For these data, a simple, automated check was made to identify gross errors in the data from the automatic weather stations by identifying values outside prescribed bounds. The bounds for the variables used in this project are given in Table 8.1.

Table 8.1 Bounds used for quality control checks on data from an automatic weather station

Variable	minimum	maximum
Downward global solar radiation (W m^{-2})	-5	1050
Net longwave radiation (W m^{-2})	-100	20
air temperature (ºC)	-10	35
wet bulb temperature (ºC)	-10	25
relative humidity (%)	25	105
wind speed (m s^{-1})	0	18
soil heat flux (W m^{-2})	-50	50
Rainfall (mm h^{-1})	0	50

There is also an AWS at CEH Wallingford, a few kilometres outside the Pang/Lambourn catchments, so further quality control was based mainly on comparing the output of particular sensors between these three stations. Generally, this consisted of comparing time series manually by examining the data from the different stations on the same graph and checking that the ‘patterns’ of fluctuations looked reasonable. This was easiest for anything with a strong diurnal signal, e.g. air temperature, soil heat flux and solar radiation. Comparisons were also made using scatter plots and look for outliers from the 1:1 line. A further check was made by comparing plots of the running cumulative totals.

Where a single value was found to be in error for variables which do not have rapid fluctuations, e.g. air temperature, it was replaced by the average of the value preceding the erroneous value and that succeeding. On all other occasions, the erroneous readings were replaced by those from the other AWS in the catchment corrected by factors determined using a linear regression for that variable from the two stations.

The exception to this procedure was relative humidity. It was apparent that the relative humidity readings from the station at Sheepdrove Farm (PL21) often exceeded 105% and could be as high as 125%, i.e. physically impossible. This suggested that there was a problem with the calibration of this sensor carried out by the manufacturer. There was no feasible method of determining the true calibration and, because relative humidity is generally conservative over the distances involved in the catchments, the entire data set from the Frilsham Meadow station was inserted in that of Sheepdrove Farm.

8.2.2 Manual weather station

Manual daily meteorological measurements consist of sunshine hours, average wind speed or run, average air temperature, rainfall and either relative humidity or wet and dry bulb temperatures. The downward solar radiation and net longwave radiation were calculated using the methods described by Thompson *et al*. (1981) from the measurements of sunshine hours, which had been quality controlled by ensuring that the measurements was not greater than the total daylight hours for that day. The wet and dry bulb temperatures were used to calculate relative humidity using the equations given by Monteith and Unsworth (1990).

These data were quality controlled and infilled using the same methods as described above for the AWS data except that it was not possible to compare the data from one station with any other, due to different time periods of data and the large distances between sites.

8.3 Evaporation

At the two LOCAR sites, actual evaporation was calculated as the residual of the surface energy balance using measurements of sensible heat flux by eddy correlation, net radiation (DRN-301, ELE International Ltd, Hemel Hempstead, UK) and soil heat flux (HP01, Hukseflux Thermal Sensors, Delft, NL) over Grass 1. The eddy correlation system consisted of a Solent R3 Research Anemometer (Gill Instruments Ltd., Lymington, UK) with the mean of five (100 Hz) samples of the three wind speed components and sonic temperature output at 20 Hz to a Campbell CR23X datalogger, sampling at 10 Hz. The cross-correlations were computed on the datalogger using an auto-regressive running mean (with time constant of 500 s) similar to (Shuttleworth and Gash, 1988), and their means and standard deviations logged every hour. This hourly data was then later processed on a PC in the laboratory to apply: an improved sonic temperature calibration; horizontal and vertical coordinate rotations(Aubinet and Grelle, 2000); the calculation of the sensible heat flux (including moisture correction of (Schotanus and Nieuwstadt, 1983); and the Moore (1986) frequency response correction.

The actual evaporation data were quality controlled, mainly by comparing the values against Penman-Monteith potential evaporation (PE) calculated using the method and parameters of Allen *et al*., 1998. Where data were missing or failed the quality control, they were infilled using the Penman-Monteith PE corrected by a linear regression between the actual evaporation and Penman-Monteith PE for a period of a few days before and after the missing data.

Potential evaporation was calculated from the meteorological data using the methods and parameter values given by Allen *et al* (1999)

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List of abbreviations

AWS	automatic weather station
FAO	Food and Agriculture Organisation of the United Nations
FRL	four root layer (soil water model)
LOCAR	Lowland catchment research (Natural Environment Research Council programme)
MOSES	Met Office surface energy scheme
NSRI	National Soil Resource Institute
RMSE	root mean square error

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