Constraining recharge and groundwater models with HydEOmex soil moisture observations

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1. Introduction

Estimation of groundwater recharge has underpinned a wide variety of groundwater resource and quality assessments within the UK at a range of scales. For example, there are many studies that have quantified time-varying recharge rates in order to model the transport of diffuse and point-source pollutants from the land surface, through groundwater systems to receptors such as rivers and abstraction boreholes (e.g. Stuart et al., 2006; Wilby et al., 2006; Jackson et al., 2007; Cuthbert et al., 2013; Ascott et al., 2016; Wang et al., 2016).

Groundwater recharge estimation is, of course, central to groundwater resource evaluation and catchment management (Environment Agency, 2011), including the estimation of sustainable groundwater abstraction licences (Environment Agency, 2013), predominantly undertaken by the UK's environmental regulators. At the scale of a UK regional aquifer (approximately 100-2500km^2) estimates of recharge have generally been evaluated by constructing catchment water balances, but also by assessing the performance of regional groundwater models driven with simulated recharge time-series (Quinn et al., 2012). Catchment boundaries used to construct water balances have not always coincided with those of groundwater systems, therefore the use of regional groundwater flow models to constrain estimates of groundwater recharge has become popular within the UK (Shepley et al., 2012).

Because recharge can only be measured directly at the point scale, and even then with difficulty, regional groundwater flow models have often been used as the only means to evaluate recharge estimates. However, it is not uncommon for both the parameters of recharge and groundwater flow models to be adjusted at the same time during model calibration to obtain a good "fit" to the state variables that can be measured: principally *groundwater levels and river flows*.

Recharge models typically simulate soil drainage, or *potential recharge*, by conceptualising the surface infiltration, evaporation, runoff, and drainage processes of the soil store. Many different types of recharge model, of varying degrees of complexity, have been applied (e.g. Finch, 1998; Heathcote et al., 2004; Sorensen et al., 2014), most of which include a variable that describes the saturation of the soil; often expressed as a *soil moisture deficit* (SMD) with respect to a *field capacity* (FC), or as a volumetric water content. Examples in which soil water contents simulated by recharge models used to drive *regional groundwater models* have been compared to observations of soil moisture are difficult to identify in the literature. Studies which consider aspects of this problem include Crow et al. (2005), Brunner et al. (2007), Montzka et al. (2012), and Albergel et al. (2012), but the specific task of assimilating soil moisture observations, whether derived from instruments installed in the soil (e.g. tensiometers or neutron probes) or remotely sensed, into distributed recharge and groundwater models does not appear to have been considered.

Recently new spatial datasets have become available due to the development and application of remote sensing methods to monitor soil moisture. Many of these datasets are derived from satellite remote sensing (at a resolution of ~1km), but in-catchment instruments are now also generating time-series of soil moisture at the field-scale (approximately 100m). These new datasets provide the opportunity to evaluate recharge models used to drive regional groundwater flow models, and to constrain their parameter values and outputs. In this study we investigate the use of new remote-sensed soil moisture data products to do this, and consider their value to the groundwater modelling community. We do this using very simple recharge and groundwater models calibrated and evaluated against observed soil moisture content and groundwater level data.

2. Data and methodology

2.1. Study site

We simulate the soil moisture content and potential recharge at Warren Farm (also referred to as Sheepdrove Farm), Berkshire, and the groundwater level time-series at the nearby Stancombe Farm observation borehole (Figure 1). Warren Farm is one of four "recharge sites" at which infrastructure was installed to measure soil moisture and other environmental variables, as part of the Lowland Catchment Research (LOCAR) programme funded by the Natural Environment Research Council (Adams et al., 2003; Ireson et al., 2006; Wheater et al., 2007).

Warren Farm and Stancombe Farm are located within the Lambourn catchment, a Chalk catchment overlain by superficial Clay-with-Flints Formation in places, and Palaeogene sands, silts and clays towards its lower reaches. Land cover is dominated by cereals and grassland, with woodland on some steeper slopes. The Warren Farm site is covered by grass and consists of a thin 0.2m Andover Series soil (Avery, 1980), including flints, on top of weathered chalk which grades into consolidated chalk between depths of 1 and 3m.

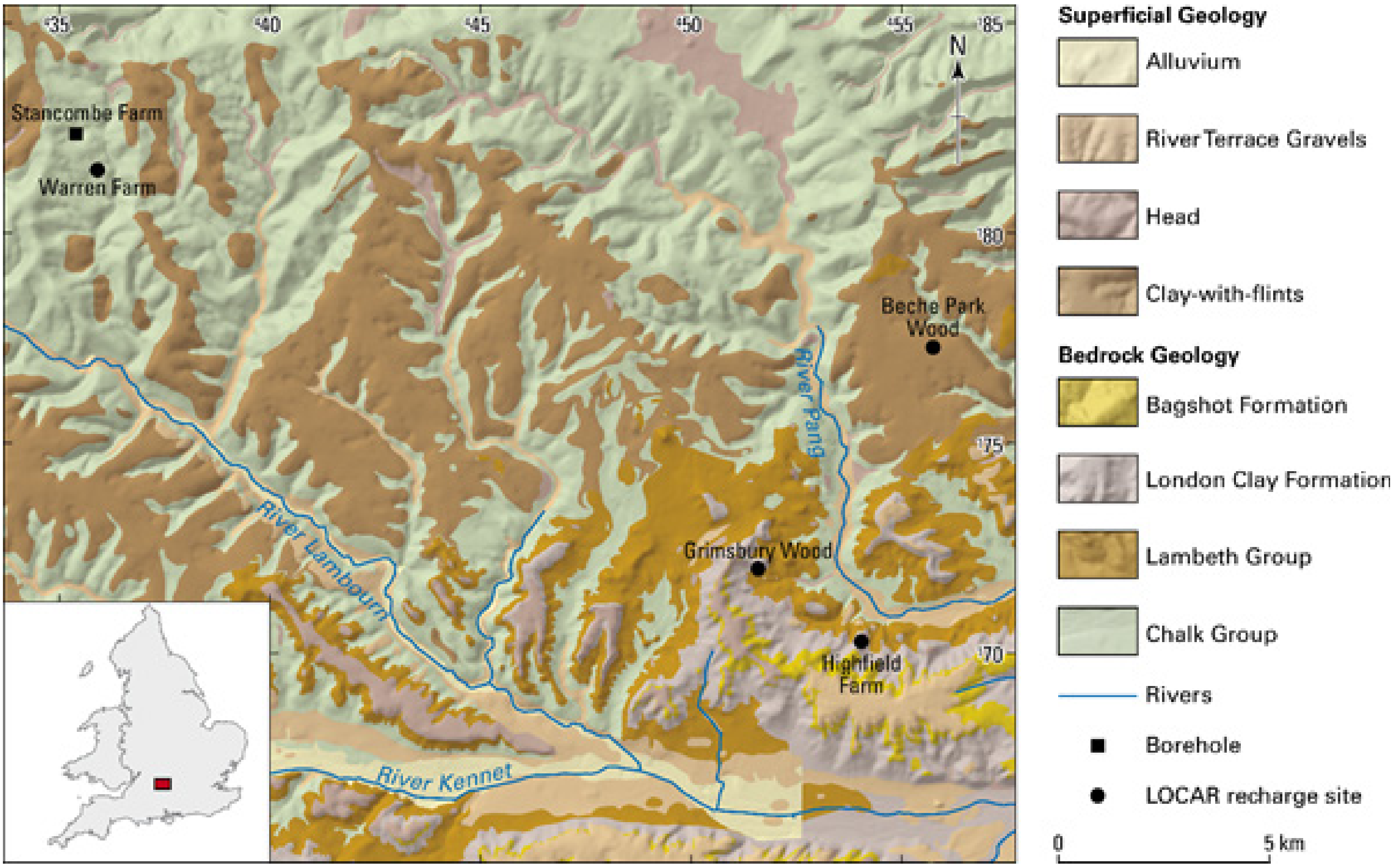

Figure 1 *Location of Warren Farm recharge site and Stancombe Farm observation borehole within the Lambourn catchment.*

2.2. Observational data

Rainfall

A daily rainfall record is available for Warren Farm based on measurements from a weighing precipitation gauge at the site. Over the period 1 November 2013 to 31 December 2014 the total rainfall was 1164mm; 2.73mm/day on average.

Potential evapotranspiration

A daily potential evapotranspiration (PET) series was calculated using the Hargreaves-Samani equation (Luo et al., 2014) based on meteorological observations from the automatic weather station at Warren Farm (daily minimum and maximum temperature, extraterrestrial radiation). This series was then scaled so that monthly mean totals were equivalent to those from MORECS (Hough and Jones, 1997). Over the period 1 November 2013 to 31 December 2014 the calculated total PET was 327mm; 0.77mm/day on average.

Soil moisture

Time-series of soil moisture for Warren Farm are available from three sources: (i) in situ monitoring using sensors installed in the soil, (ii) a cosmic ray soil moisture (COSMOS) sensor, and (iii) satellite derived observations.

DIGITAL TIME DOMAIN TRANSMISSOMETRY (TDT) SENSORS

Soil moisture has been measured at Warren Farm at hourly intervals since 24 October 2013 using two digital time domain transmissometry (TDT) sensors installed in the soil at depths of 10, 15, 40, and 65cm. These observed series were aggregated to derive a bulk moisture content for the soil assuming the measurements at a depth of 65cm represent the interval between 52.5 and 77.5cm. This aggregated series is plotted in Figure 2.

COSMOS

The cosmic ray soil moisture (COSMOS) sensor at Warren Farm is one of the network of these sensors installed and run by the Centre for Ecology and Hydrology (CEH, 2016a). Each COSMOS instrument uses cosmic rays to sense soil moisture over an area up to 700m in diameter, and to a depth of up to 70cm. However, these estimates for area and depth are likely maxima, and decrease with water content so that in a wet soil the effective depth reduces to 15cm.

Daily mean values of the volumetric pore water content (%) derived from the COSMOS instrument were provided by CEH for the period November 2013 to January 2016 (Figure 2).

SATELLITE OBSERVATIONS

Satellite-derived soil moisture data were obtained from the European Space Agency's Climate Change Initiative (ESA CCI) compressed dataset (Liu et al. 2011, 2012; Wagener et al., 2012). This dataset provides values of soil moisture as a percentage of saturation, on a 1km grid over the UK, and a daily time-step for the period 2010-2014. Further information about these data and their use in the HydEOmex project are provided in the accompanying report by Williams and Quaife (2016).

Satellite microwave sensors provide estimates of soil moisture in a thin surface layer (0.5-5cm), which is directly exposed to the atmosphere and the sun. Consequently it must be noted that satellite measurements represent a soil layer where soil moisture content is likely to be more variable than deeper part of the soil column.

COMPARISON OF SOIL MOISTURE OBSERVATIONS

Soil moisture time-series for all three sets of observations are plotted in Figure 2. Given the depths of the in situ measurements, and the characteristics of the COSMOS and ESA CCI measurements, the series derived from the soil probes is likely to represent the greatest depth of soil, and the satellite data the shallowest. This is consistent with the variability of the different time-series with the TDT sensor data exhibiting the least daily variability, particularly during dry periods. As would be expected, given it represents only up to the top ~5cm of the soil, the ESA CCI data exhibits the greatest variability. Whilst there are obvious differences between the datasets the monthly to seasonal variability in the three series is in reasonable agreement, which suggests potential value in using satellite-remote sensed soil moisture to constrain spatio-temporal estimates of groundwater recharge.

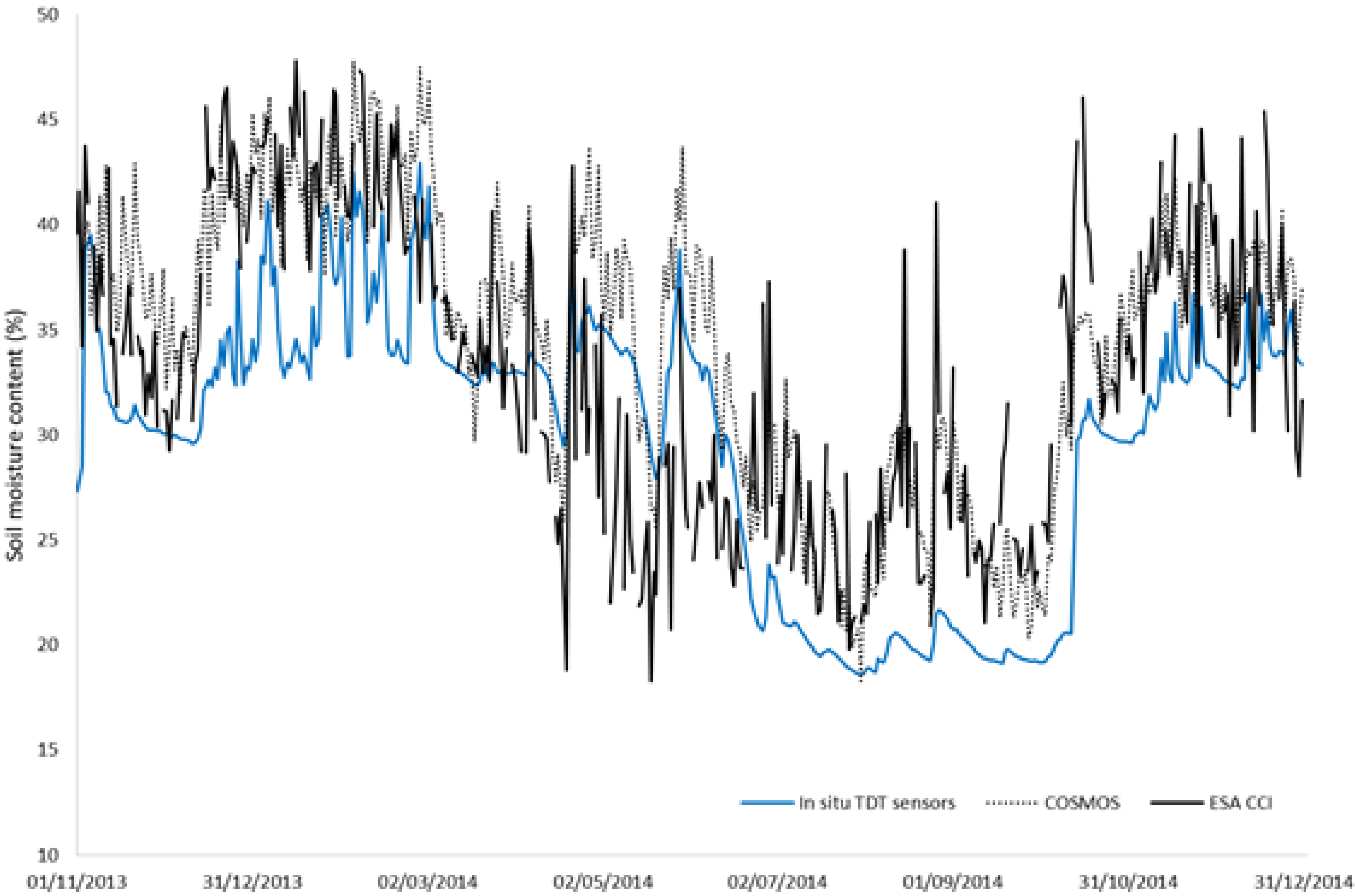

Figure 2 *Soil moisture time-series derived from in-situ TDT sensors, the COSMOS instrument and ESA CCI.*

Groundwater levels

There is no observation borehole at Warren Farm. However, approximately weekly measurements are taken in the open observation borehole at Stancombe Farm, 970m away (Figure 1). Over the period November 2013 to January 2016 groundwater levels fluctuated here between 48.2 and 23.6 m below ground level (134.0 to 158.6 m aOD). The elevation of the land surface at Warren Farm is approximately 6m higher than at Stancombe Farm, and the mean groundwater level, derived from contoured historical measurements from observation boreholes, is estimated to be approximately 5m lower, based on contouring of groundwater level measurements from surrounding observations boreholes (e.g. see Figure 4 in Jackson et al., 2011). Consequently, groundwater levels are likely to be approximately 11m deeper at Warren Farm.

2.3. Modelling methodology

Potential recharge and groundwater levels are simulated using the AquiMod code (Mackay et al., 2014). AquiMod is a simple, lumped-catchment groundwater model that simulates groundwater level time-series at a point by linking simple algorithms of soil drainage, unsaturated zone flow and groundwater flow. It takes time-series of rainfall and potential evapotranspiration as input, and produces time-series of soil moisture content, potential recharge and groundwater level. AquiMod facilitates the use of multiple different algorithms (model structures) to simulate these variables.

AquiMod is not calibrated against an objective function through the optimisation of model parameter values. Instead, Monte Carlo simulations are performed to identify behavioural models that meet a pre-defined error criterion. Prior to each simulation within the Monte Carlo run, model parameter values are randomly sampled from a uniform distribution, given lower and upper limits.

Simulation of potential recharge

To simulate potential recharge and soil moisture we use the soil moisture accounting procedure (SMAP) of Mathias et al. (2014), which uses an explicit Euler time-stepping scheme to solve the integrated mass conservation equation:

$$\frac{d\Theta}{dt} = q_r - q_{ro} - q_d - E_a \qquad \text{Equation 1}$$

where Θ is the volumetric soil moisture content, q_r is the net rainfall rate [LT^{-1}], q_{ro} is the surface runoff [LT^{-1}], q_d is the soil drainage rate [LT^{-1}], and E_a is the actual evaporation [LT^{-1}]. The last three terms of Equation 1 depend on the soil moisture content, for which Mathias et al. (2014) describe the functional relationships. In total the model requires the specification of values for 10 parameters, five of which are adjusted during the Monte Carlo run.

Simulation of groundwater levels

Groundwater levels are simulated by AquiMod using the simple algorithm presented by Park and Parker (2008). This solves for the groundwater level, h, at time-step i+1 based on the following equation:

$$h_{i+1} = h_{min} + h_i exp(k\Delta t_i) + \frac{R_i [exp(k\Delta t_i)-1]}{kS_y} \qquad \text{Equation 2}$$

where h_{min} is the minimum groundwater level [L], k is a residence time parameter [T^{-1}], Δt_i is the length of time-step i [T], R_i is the recharge [LT^{-1}] over the time-step, and S_y is the specific yield of the aquifer.

Model application

We investigate whether the availability of remote sensed soil moisture data is useful to constrain estimates of potential recharge made using AquiMod, and therefore, by inference, regional groundwater models. Here we undertake four Monte Carlo runs (Table 1). When considering the COSMOS soil moisture we set the thickness of the SMAP component's soil store to 400mm, assuming that this is the depth of soil over which the COSMOS instrument measures water content. We recognise that the depth of soil over which COSMOS instruments measure soil moisture varies with saturation content (up to 750mm; CEH, 2016b), and therefore it could be suggested that a soil moisture model that discretises the soil in the vertical should be applied. However, given the aim of this modelling is to test the benefit of new soil moisture datasets in the application of widely applied single-layer soil moisture accounting models we consider this a reasonable compromise.

When considering the ESA CCI data we make the assumption that the derived soil moisture observations are representative of a 200mm soil and set the modelled soil depth accordingly. This contradicts our previous statement that satellites only measure soil moisture over a thin surface layer, and we recognise that this will introduce error. However, the simulation of such a thin soil is not practicable with models such as SMAP model when using daily driving stresses, and it is for this reason that we increase the modelled soil depth.

First, we setup AquiMod to include both the SMAP and saturated groundwater components (Table 1: Runs 1a and 1c). Daily potential recharge calculated by the SMAP component was used to drive the saturated groundwater component to simulate the Stancombe Farm groundwater hydrograph. The values of the parameters of both the SMAP and saturated groundwater components were sampled during the Monte Carlo run. We evaluated model performance by calculating the fit to the observed groundwater level time-series using the Nash-Sutcliffe Efficiency (NSE) score:

$$NSE = 1 - \frac{\sum_{t=1}^{n} (y_o^t - y_m^t)^2}{\sum_{t=1}^{n} (y_o^t - \overline{y_o})^2} \qquad (1)$$

where y_o and y_m are the observed and modelled values, respectively.

We defined a threshold NSE of 0.5, above which a model parameter set was deemed to be acceptable or *behavioural*. For each acceptable model we calculated the total potential recharge over the simulation period 1 November 2013 to 31 January 2014.

Second, we setup AquiMod to include only the SMAP module and evaluated performance against the remote sensed soil moisture content (Table 1: Runs 1b and 1d). We accepted parameter sets that produced an NSE of 0.5 and above when comparing the simulated and observed soil moisture content. For each acceptable model we calculated the total potential recharge over the simulation period 1 November 2013 to 31 January 2014.

Table 1 *Monte Carlo run summary*

Run	SMAP	Saturated groundwater	NSE calculated using
1a	On (400 mm soil)	On	Groundwater level
1b	On (400 mm soil)	Off	COSMOS soil moisture
1c	On (200 mm soil)	On	Groundwater level
1d	On (200 mm soil)	Off	ESA CCI soil moisture

3. Results

Evaluated against the observed groundwater levels, Monte Carlo Run 1a produced 2943 behavioural simulations from the ensemble of 100,000 simulations, with a maximum NSE of 0.83 (Figure 3). Total potential recharge over the 426-day period varied between 459 and 1130mm (1.08 to 2.65mm/day) (Figure 4a). The total potential recharge for the best 10 simulations ranged between 505 and 681 (1.19 to 1.60mm/day).

Evaluated against soil moisture content derived from COSMOS, Monte Carlo Run 1b produced 6387 behavioural simulations from the ensemble of 100,000 simulations, with a maximum NSE of 0.83.

Simulated total potential recharge varied between 505 and 808mm (1.19 to 1.90mm/day) (Figure 4b). The total potential recharge for the best 10 simulations ranged between 539 and 608 (1.27 to 1.43mm/day). The COSMOS observations and soil moisture content simulated by the best Run 1b model are shown in Figure 5. SMAP produces a reasonable fit to the observed soil moisture but does not capture the measured short time-scale (daily) variability.

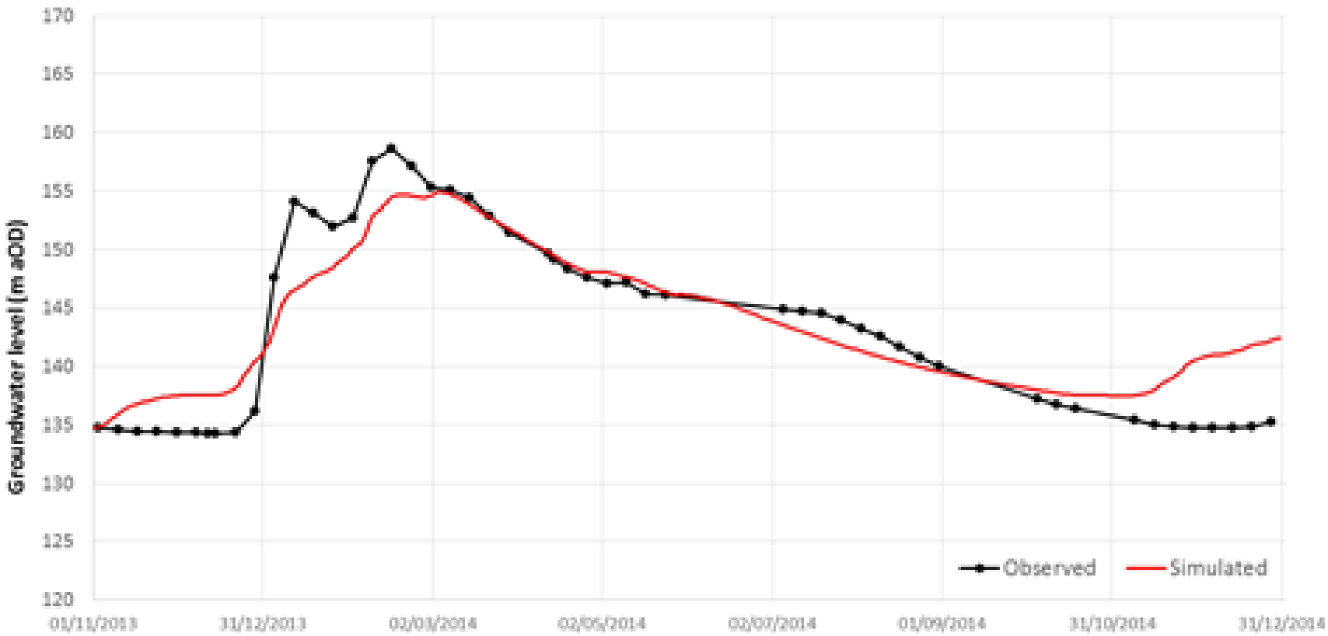

Figure 3 *Observed and simulated (by best model) groundwater level (400 mm soil)*

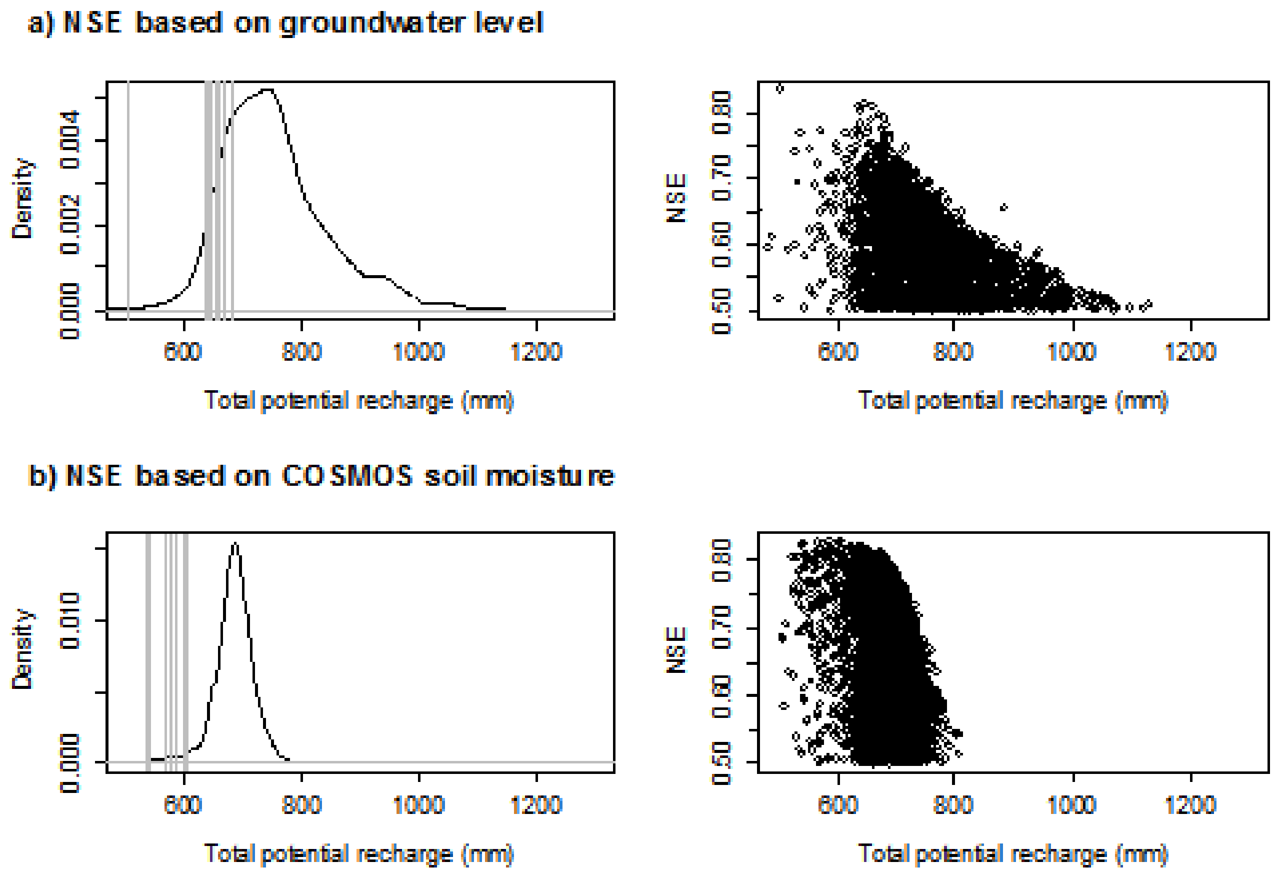

Figure 4 *Distribution of simulated recharge rates for each behavioural model (400 mm soil) when evaluated using a) groundwater level and b) COSMOS soil moisture content. Vertical grey lines represent the 10 simulations obtaining the highest NSE scores.*

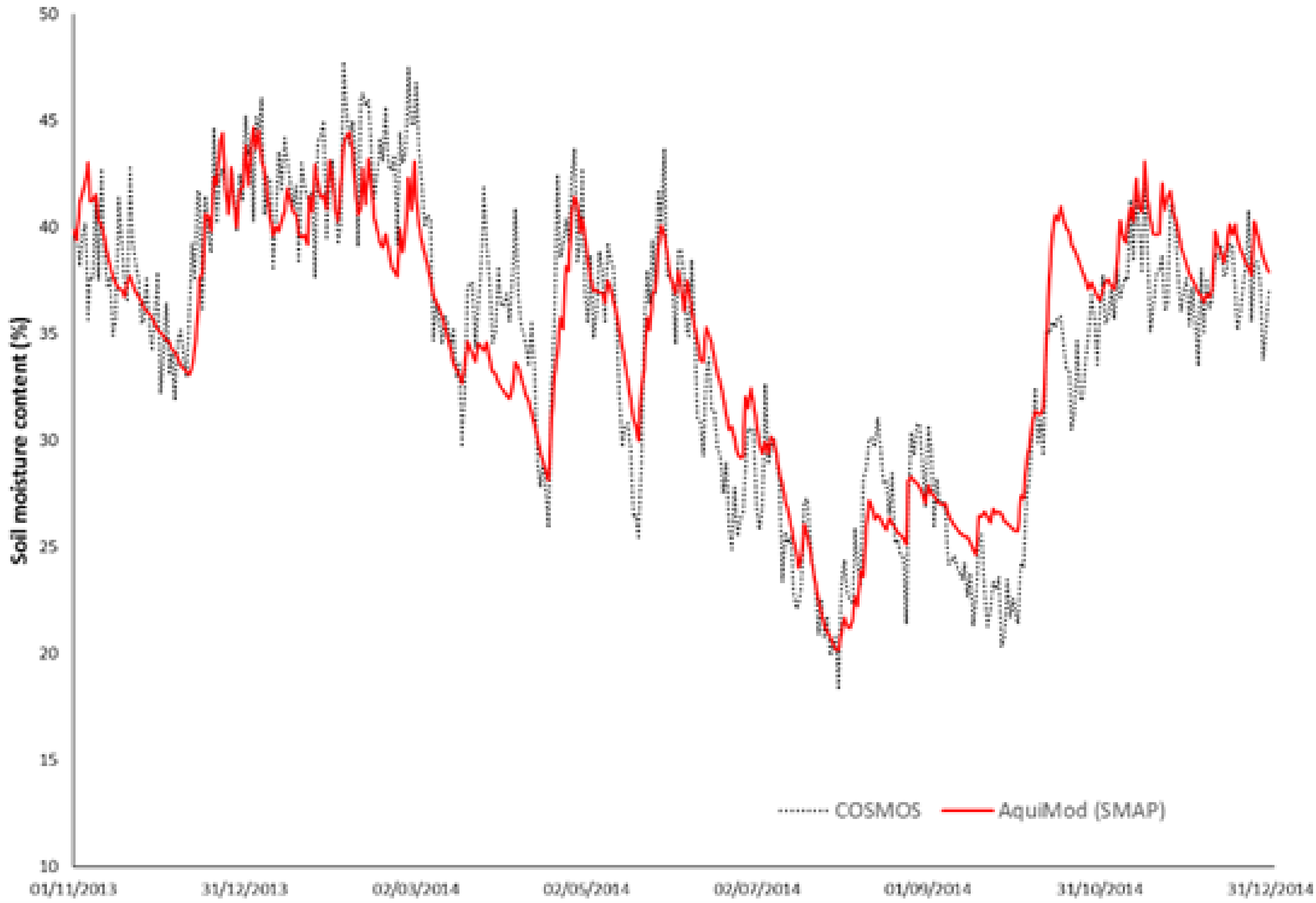

Figure 5 *Observed COSMOS and simulated (Run 1b) soil moisture content for best model (NSE = 0.83).*

Evaluated against the observed groundwater levels, Monte Carlo Run 1c produced 3357 behavioural simulations from the ensemble of 100,000 simulations, with a maximum NSE of 0.72. Total potential recharge varied between 493 and 1219mm (1.16 to 2.86mm/day) (Figure 6a); the higher value is greater than the total rainfall and therefore the soil drained in these simulations. The total potential recharge for the best 10 simulations ranged between 629 and 802 (1.48 to 1.88mm/day).

Evaluated against soil moisture content derived from ESA CCI, Monte Carlo Run 1d produced 220 behavioural simulations from the ensemble of 100,000 simulations, with a maximum NSE of 0.57. Simulated total potential recharge varied between 556 and 745mm (1.31 to 1.75mm/day) (Figure 6b). The total potential recharge for the best 10 simulations ranged between 562 and 626 (1.32 to 1.47mm/day). The ESA CCI observations and soil moisture content simulated by the best Run 1d model are shown in Figure 7. The fit to the observations is reasonable, though the model does not capture much of the daily variability.

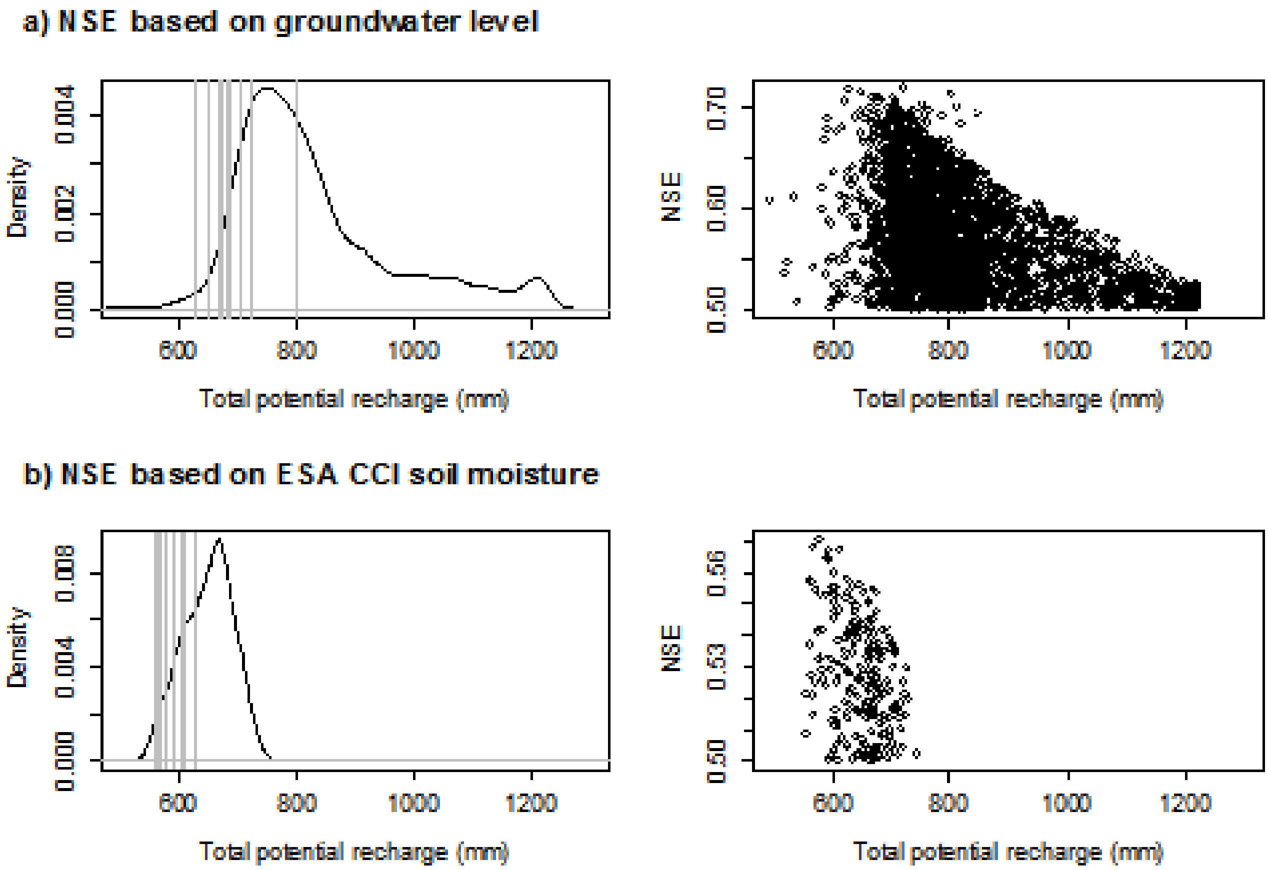

Figure 6 *Distribution of simulated recharge rates for each behavioural model (200mm soil) when evaluated using a) groundwater level and b) ESA CCI soil moisture content. Vertical grey lines represent the 10 simulations obtaining the highest NSE scores.*

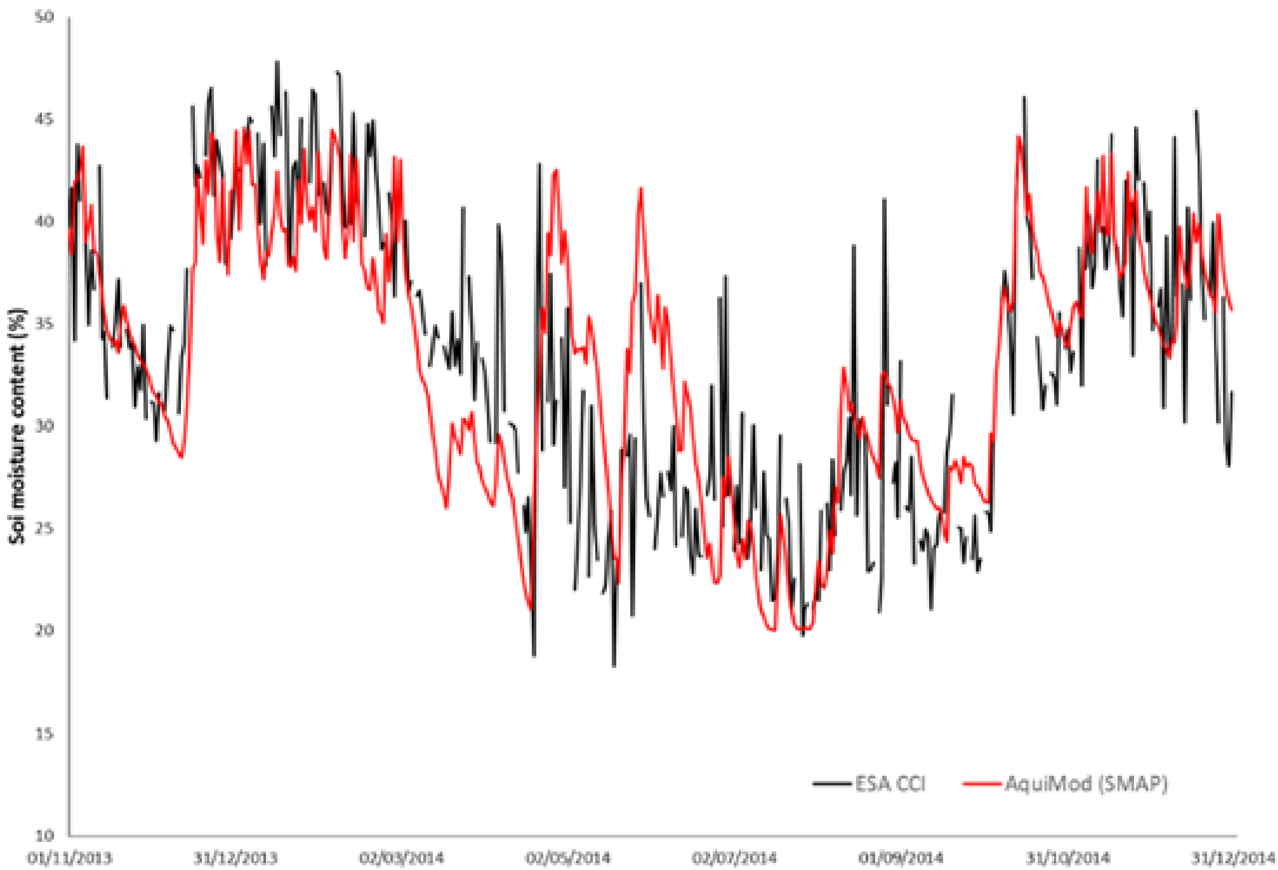

Figure 7 *Observed ESA CI and simulated (Run 1d) soil moisture content for best model (NSE = 0.57).*

Table 2 *Summary of simulated total potential recharge (mm) from Monte Carlo runs*

Run	NSE calculated using	All behavioural simulations		Best 10 simulations	
		Min	Max	Min	Max
1a	Groundwater level	459	1130	505	681
1b	COSMOS soil moisture	505	808	539	608
1c	Groundwater level	493	1219	629	802
1d	ESA CCI soil moisture	556	745	562	626

4. Conclusions

The saturated groundwater component of AquiMod, which has been used to simulate the groundwater Stancombe Farm groundwater hydrograph is a very simple model and only represents a point in space. It does not, of course, incorporate the complexity of a distributed groundwater model used to simulate a regional groundwater system. However, it has been driven by potential recharge generated by a soil moisture accounting model (SMAP) similar to those routinely used to produce such inputs to regional groundwater models.

We have shown that AquiMod can reproduce the observed groundwater level hydrograph reasonably well given the wide range of simulated total recharge values produced by an ensemble of behavioural AquiMod models. This is consistent with the concept of equifinality (Beven, 2006), which is the basis for the interpretation of AquiMod modelling results; the two parameters of AquiMod's saturated groundwater component (residence time and specific yield) allow the model to fit the groundwater level data equally well given many different recharge time-series. Consequently, when calibrating against groundwater level (only) the model is not sensitive to the magnitude of the recharge series. Whilst the modelling undertaken here is simple, the same issue occurs in regional groundwater modelling, where, as described in the introduction, it is not uncommon for both the parameters of recharge and groundwater flow models to be adjusted at the same time during model calibration to obtain a good "fit" to the state variables that can be measured: principally *groundwater levels and river flows*.

Comparison of soil moisture measurements made using sensors installed in the soil with remote sensed observations derived from the COSMOS instrument and ESA CCI, has shown that they are in reasonable agreement. Although we found that, for this very simple model compared against one groundwater level hydrograph, the use of the COSMOS and ESA CCI observations has had no influence on the accuracy of simulated groundwater levels, it has enabled the estimates of potential recharge to be constrained, and reduced the range (upper minus lower values) of the distribution derived from the ensemble of simulated total potential recharge at Warren Farm over the 426-day period of simulation. For example as described in Table 2, when ignoring the soil moisture data, estimates of total potential recharge varied from 459 to 1219mm. When the model was evaluated against the COSMOS data, estimates varied between 505 and 808mm based on all behavioural SMAP models and between 539 and 608mm based on the best 10 simulations. This compares to a total effective precipitation (rainfall minus potential evapotranspiration) of 641mm over this period.

In contrast to the simple modelling of a groundwater level time-series undertaken here, regional groundwater models simulate groundwater water balances. As described previously, regional groundwater models of aquifers have typically only been calibrated against groundwater level hydrographs from observation boreholes, and against river flows time-series. We have illustrated that the use of remote sensed soil moisture data enables the uncertainty associated with estimates of potential recharge to be reduced. Soil moisture data have not been used in this way within regional modelling studies within the UK. However, if this were the case, it is expected that uncertainty in the parameterisation of distributed groundwater models could be reduced.

Whilst we conclude, from this short study, that remotely-sensed soil moisture datasets are of value in groundwater modelling, our findings are limited because of the simplicity of the groundwater model used, and its evaluation against a single groundwater level time-series. To more thoroughly investigate the benefits derived from the use of remotely-sensed soil moisture products, we suggest using them in the calculation of spatio-temporally varying recharge for a distributed groundwater model, which is then evaluated against multiple time-series of both groundwater levels and river flows. For example, it would be worthwhile assessing the outcomes of assimilating soil moisture observations into groundwater model simulations, which are then used to make forecasts.

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