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Some measures of uncertainty in a cropping system model for predicting hydrology and erosion

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Abstract: The soil water balance model PERFECT was developed and validated on a number of experimental sites throughout Queensland. This model, and variations of, has been widely used to assess the impacts of crop and fallow management on hydrology, sediment generation, deep drainage, crop growth and yield. In recent years, PERFECT has been applied spatially to model the environmental impacts of management at the catchment scale, often with little data available for calibration and validation.

Uncertainty in these spatial implementations of PERFECT come from a variety of sources – from the spatial data that go into representing model scenarios, to climate inputs, parameterisation of soils and management systems and the structure of the model itself. Formal assessments of each of these sources of uncertainty are lacking, and before the spatial uncertainty of these models can be addressed the fundamental uncertainty surrounding parameterisation and model structure should be addressed. This paper attempts to explore predictive uncertainty in PERFECT, and predictive error variance for a particular calibration case, using PEST software with data and an existing parameter set from an experimental site at Greenmount, southern Queensland, Australia.

Eighteen parameters were included in the analysis, and four sets of measured data – runoff, soil water, deep drainage and erosion. The information content of the observations was sufficient for seven dimensions of parameter space to be determined; half the parameters could be identified to some degree. Parameter identifiability appears to be driven by the limited range of processes captured in the data.

The contributions of parameters to predictive uncertainty varied according to the prediction of interest, as did the importance of the different observation datasets to reducing uncertainty. Uncertainty bounds of key predictions of runoff, erosion and deep drainage were as good as, or better, than expected (e.g., ± 2.1 mm runoff for one large event, ± 10.2 mm for total runoff volume in the four-year validation period), suggesting that more sources of uncertainty could be identified in future analyses. This study has provided valuable information on the uncertainty in PERFECT which was not previously available, and has raised a number of questions which could be explored in future studies.

Keywords: *predictive uncertainty, PERFECT, PEST, runoff, soil water balance, erosion*

1. INTRODUCTION

The cereal cropping zone of southern Queensland, Australia, has long been the focus of research into the impacts of land management on hydrology and soil loss. Long-running experimental sites were established in this region in the 1970s and 1980s to assess the impact of management practices on hydrology, erosion and production in cropping systems. At the same time, an integrated model was developed to better understand these interactions. This model, PERFECT (Littleboy et al. 1989, 1999), has since been widely validated on experimental sites around Queensland (e.g., Littleboy et al. 1989, 1992, 1996; Freebairn et al. 1991; Thomas et al. 1995; Thornton et al. 2007). PERFECT, and its derivatives, remain in common use for site-based modelling of production, hydrology and erosion. In recent years, these models have been applied spatially to simulate the environmental impacts of management at the catchment scale, often with little or no data for calibration and validation.

PERFECT uses a range of input parameters pertaining to crops, management, soil, hydrology and erosion, some of which may be derived from field measurement or surrogate (pedo-transfer) models, and others by rules-of-thumb or calibration. Throughout the years of its application, there has been no formal assessment of model uncertainty, excepting a local sensitivity analysis reported in the original PERFECT manual (Littleboy et al. 1989). In fact, there is little record in the literature of uncertainty assessment for agricultural systems models. Notable exceptions include Wang et al. (2005) on uncertainty in corn yield and soil organic carbon predictions in EPIC using the GLUE methodology, Pathak et al. (2007) on the uncertainty of a new cotton model in CROPGRO using global sensitivity analysis, and several studies on uncertainty of crop model predictions due to varying climate data inputs (e.g., Nui et al. 2009, Rivington et al. 2006).

With recent moves to apply PERFECT to complex spatial scenarios, predictive uncertainty is emerging as an issue. Uncertainty in spatial implementations of PERFECT come from a variety of sources – from the spatial data that go into representing model scenarios, to climate inputs, parameterisation of soils and management systems and the structure of the model itself. While spatial modellers are aware that the application of these site-based models across complex landscapes will involve substantial error, there is an expectation that they can discriminate between the range of environmental conditions mapped out across a landscape. Before the spatial uncertainty of these models can be addressed, the fundamental uncertainty surrounding parameterisation and model structure should be assessed. This paper attempts to explore predictive uncertainty in PERFECT, and predictive error variance for a particular calibration case, using PEST software (Doherty 2008) with data and an existing parameter set from an experimental site in southern Queensland.

2. METHODS

2.1. The PERFECT Model

PERFECT is a daily time-step biophysical model which simulates the dynamics of plant growth, soil water balance, ground cover, soil erosion and management in a cropping system. PERFECT simulates a one-dimensional water balance, coupled with a dynamic crop model and a simple erosion algorithm. Thorough descriptions of the components of PERFECT can be found in Littleboy et al. (1999).

2.2. Study Site and Data

Uncertainty in PERFECT was explored using experimental data, and the results of previous modelling efforts, from a site at Greenmount, south of Toowoomba in southern Queensland, Australia (Freebairn and Wockner 1986). This site is considered representative of much of the cropping land of the eastern Darling Downs, and has a relatively long data record compared to most other experimental sites around Queensland. Several contour bays were instrumented at the site; the dataset used in this study is a composite of bays forming a continuous record under wheat with a burnt stubble treatment.

Data collected at Greenmount are described in Freebairn and Wockner (1986). The common period of record for key datasets runs from 20/04/1976 to 31/12/1988. It includes runoff measured at the end of the contour bays, water contents for each soil horizon (after harvest, mid-fallow and prior to planting) and total soil movement. The study period captured a wide range of events and is considered a good representation of the site. A deep drainage rate estimate for Greenmount, of 14 mm/yr (for the period 1977 – 1996), is also available from the chloride study of Tolmie et al. (2004).

The first eight months of the record were designated as a model warm-up, while the remainder was divided into an eight year calibration period (1977 – 1984), used to condition the uncertainty matrix, and a four year validation period (1985 – 1988) to test the uncertainty of key predictions (Figure 1).

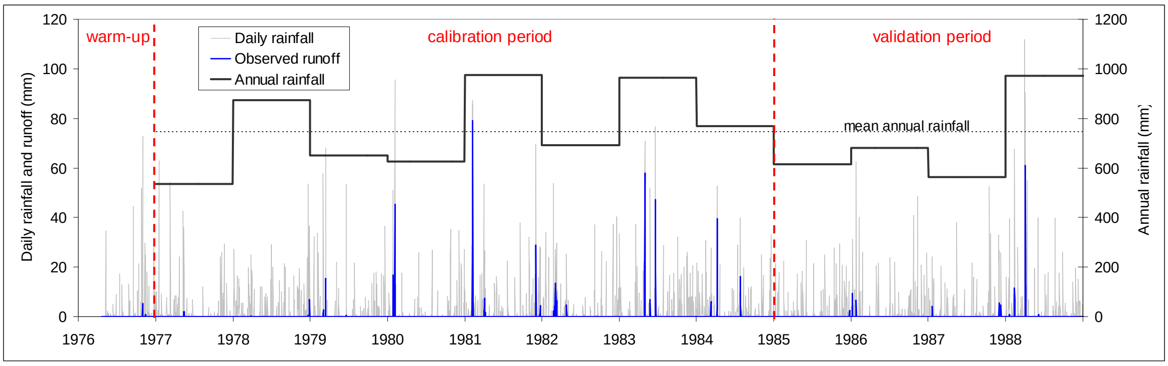

Figure 1. Measured rainfall and runoff data for Greenmount, April 1976 – December 1988.

2.3. Uncertainty Analysis

All models, by definition, are simplifications of reality. The inability of a model to simulate real systems results in some amount of predictive error, with the potential for error increasing as the structural inadequacy of the model to support a given prediction increases (Gallagher and Doherty 2007). Noise in calibration data further confounds the issue. 'Uncertainty' can be considered an intrinsic Bayesian quality, a measure of the inability of a model to simulate the true nature of a system due to these various sources of error.

Even with a model operating at a reduced resolution to reality, the information content of calibration data is often insufficient to uniquely identify all parameters in a hydrologic model (Doherty and Hunt 2009); any number of parameter sets may exist that will acceptably simulate the processes of interest. Calibrating a model is a deterministic approach that requires a unique solution be found to what is really a non-unique problem. To achieve calibration, a model must be parsimonised, further simplifying it to allow a unique parameter set to be found. In this way, the calibration process itself may add to the error of the prediction.

PEST (Doherty 2008) is a model-independent software package used for parameter estimation and predictive uncertainty analysis. PEST was first used to carry out singular value decomposition, providing an estimate of the number of dimensions of the models solution space, identifiability of each parameter in that space (i.e., the ability of observation data to constrain parameters), and relative reduction in error from each parameter due to calibration (Doherty and Hunt 2009). This analysis was carried out on the full data record from 1977 – 1988. The data were then split into the calibration and validation sets, and the PREDVAR and PREDUNC utilities were used to perform some simple linear analyses of predictive uncertainty. These provide assessments of the uncertainty of key model predictions, the contribution of each parameter to predictive uncertainty and the value of different observation data types in reducing uncertainty.

Parameter values

Saturated hydraulic conductivity, evaporation, curve number and soil erosion parameters were obtained from previous manual model calibrations (Owens et al. 2004; Littleboy et al. 1989) (Table 1). This type of information is commonly taken from an experimental site and extrapolated to similar soils for the purposes of spatial modelling. Roughness parameters, *cntil* and *rrr*, had not been calibrated but were included in this analysis to ensure a more thorough assessment of the model. These parameters were set to low values, as roughness is considered a minor driver of hydrology at this site. Parameters pertaining to soil water (air dry moisture content, crop lower limit, drained upper limit and porosity) were fixed based on the measured soil water data, and were not included in the uncertainty analysis. The soil was simulated using six layers. Crop growth was modelled using the Woodruff-Hammer wheat model using a fixed phenology algorithm; two growing season parameters (*dd_em* and *dd_an*) and two root growth parameters (*rootg* and *rootm*) were included as the most likely sources of uncertainty for simulating crop growth.

Uncertainty in the parameter values was defined by subjectively estimating possible parameter distributions, based on local knowledge of the Greenmount site and considering the known structural or theoretical bounds to each parameter. Parameter values and their distributions were log transformed during the analysis.

Observation data

Four observation data types were included in this study – daily runoff, total profile soil water, daily erosion and average annual deep drainage rate. Measurement noise was accounted for by estimating the likely error bounds for each type of observation; this was ± 2 mm for daily runoff, ± 25 mm for profile soil water, ± 3 t/ha for daily erosion and ± 3 mm for the deep drainage rate. Each observation group was then weighted to the inverse of these uncertainties.

Time series data contain some degree of autocorrelation, resulting in an information content below what may be expected from the total number of observations. This is particularly the case with episodic runoff in contour bays, where the majority of days have zero runoff – these data points provide little information to the model. In an attempt to account for temporal autocorrelation, runoff and erosion observations were only included in the analysis when they related to a rainfall event – either days that had rain, or the first day after rain. All other days in the runoff and erosion records had a zero weighting applied. For the uncertainty analyses, all observations in the validation period removed by weighting them to zero.

Table **1**. Parameters included in the analysis, their calibrated/default value and assessment of their uncertainty

Parameter	Description	Value	Expert assessed uncertainty bounds
ksat1	Saturated hydraulic conductivity (mm/hr) for each horizon	3.0	0.5 – 4.5
ksat2		1.0	0.4 – 1.2
ksat3		1.0	0.2 – 1.2
ksat4		1.0	0.1 – 1.2
ksat5		0.1	0.01 – 0.3
ksat6		0.1	0.01 – 0.2
cona	Stage II soil evaporation	3.75	3.5 – 6.5
u	Stage I soil evaporation limit (mm)	8	4 – 10
cn2	Bare soil curve number	73	60 – 80
cnred	Reduction in curve number at 100% cover	20	0 – 40
cntil	Maximum reduction in curve number due to tillage	5	0 – 20
rrr	Cumulative rainfall to remove roughness (mm)	40	25 – 200
dd_em	Degree days for crop emergence	120	90 – 150
dd_an	Degree days from anthesis to harvest	600	400 – 700
rootg	Root growth per day (mm)	13.5	8.0 – 16.0
rootm	Maximum root depth (mm)	1500	1200 – 1800
k	Soil erodibility factor	0.37	0.2 – 0.5
rill	Soil rill/interrill ratio	3.0	1.0 – 5.0

3. RESULTS

3.1. Parameter Space and Identifiability

Repeated singular value decomposition, using increasing numbers of dimensions, resulted in a major drop in error variance of key predictions at seven singular values. This indicates the likely number of dimensions of the model solution space (Doherty 2008). That is, in this case, of the eighteen dimensions of parameter space, only seven dimensions can be resolved. Parameter identifiability (the cosine of the angle between a parameter's unit vector and its projection into the solution space; Doherty and Hunt 2009) within these seven dimensions is illustrated in Figure 2. This index may vary between 0 and 1, with 0 indicating a parameter is completely un-identifiable and a value of 1 indicating it is completely identifiable, based on the available observation data. The idenfiability index, combined with the relative error reduction index, indicate that *ksat1*, *ksat2*, *cona*, *u*, *cn2*, *k* and *dd_em* are the most important parameters in terms of their contribution to predictive uncertainty.

The results in Figure 2 demonstrate that the *ksat* parameters, excepting *ksat2*, are largely unidentifiable; this may be due to the use of total profile soil water rather than horizon-based data. Parameters *cona*, *u* and *cn2*

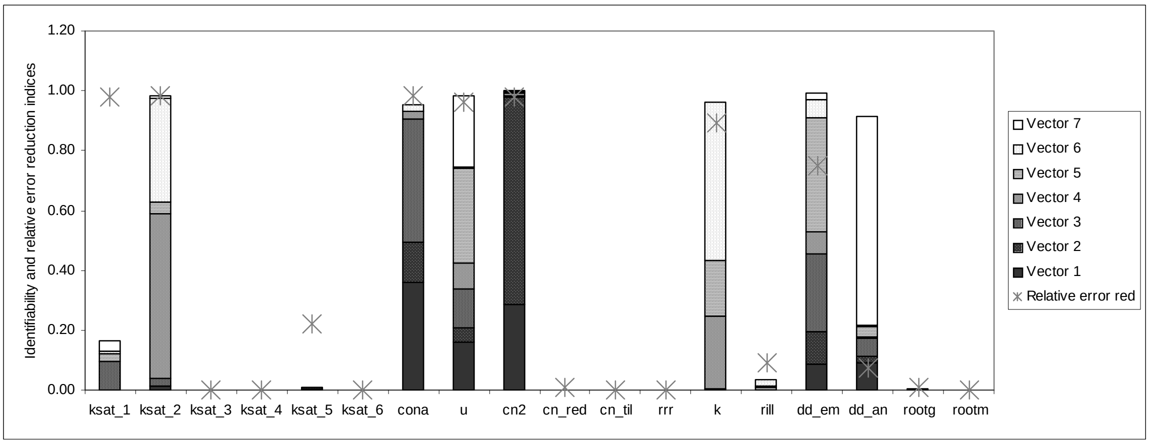

Figure 2. Parameter identifiability, and contribution of parameters to the seven dimensions of the solution space, based on observation data for the period 1977 – 1988.

are well identified, however, the other curve number parameters are completely unidentifiable. The experimental data, being for a burnt stubble treatment which is one of several fallow treatments studied at Greenmount, has a limited range of cover and tillage conditions represented in the data, thus providing little to inform the parameters relating to cover and tillage.

In the crop model, the growing season parameters are identifiable, while the root growth parameters are not. Again, this may be due to the exclusion of horizon-specific soil water data. In the erosion model, a major difference in identifiability between *k* and *rill* is reflective of the expert knowledge of these parameters and the erosion processes acting at this site. The dominance of *cn2* and *cona* on the major vectors 1-3 suggests they are the most identifiable overall.

3.2. Predictive Uncertainty

Predictive uncertainty was assessed for some long term predictions which are indicative of the type of prediction commonly required of PERFECT. These were total runoff, erosion and deep drainage for the entire validation period. Uncertainty of a daily runoff prediction (on 3/4/1988, the largest event in the validation period) was also assessed to contrast between the broad and fine temporal scales.

Uncertainty bounds on these four predictions are shown in Table 2, along with the predicted values. These results show that pre-calibration predictive uncertainty, based only on expert assessment, is high but is reduced through calibration. The uncertainty bounds of the calibrated model are within the limits expected of PERFECT; they may in fact be narrower than expected, possibly reflecting an omission in this study of other sources of uncertainty.

Table **2**. Uncertainty bounds of predictions, based on expert prior assessment of parameter uncertainty vs. based on the calibrated model

Prediction	**Predicted value**	**Uncertainty (2 st dev)**	
		Uncalibrated	Calibrated
Total runoff	269.5 mm	± 73 mm	± 10.2 mm
Total erosion	228.7 t/ha	± 69.2 t/ha	± 9.0 t/ha
Total deep drainage	53.8 mm	± 37.5 mm	± 6.8 mm
Daily runoff (3/4/1988)	59.3 mm	± 15.5 mm	± 2.1 mm

The contributions of each parameter to error variance in the calibrated model, for the four predictions, are shown in Figure 3. For both the long term and daily runoff predictions, *cn2* makes the largest contribution to predictive uncertainty. Moving from long term to daily, the *ksat* parameters make a larger contribution to uncertainty, while *rrr* and the crop parameters are of lesser importance. For the prediction of total erosion, all the hydrology parameters remain large contributors to uncertainty, reflecting the strong dependence of the erosion model on hydrology. It is interesting to note that *rill* makes no contribution to this prediction. In the prediction of deep drainage, the crop parameters are more dominant, reflecting the reliance of deep drainage predictions on the accurate simulation of soil water. The *rootm* parameter made no contribution to uncertainty for all predictions.

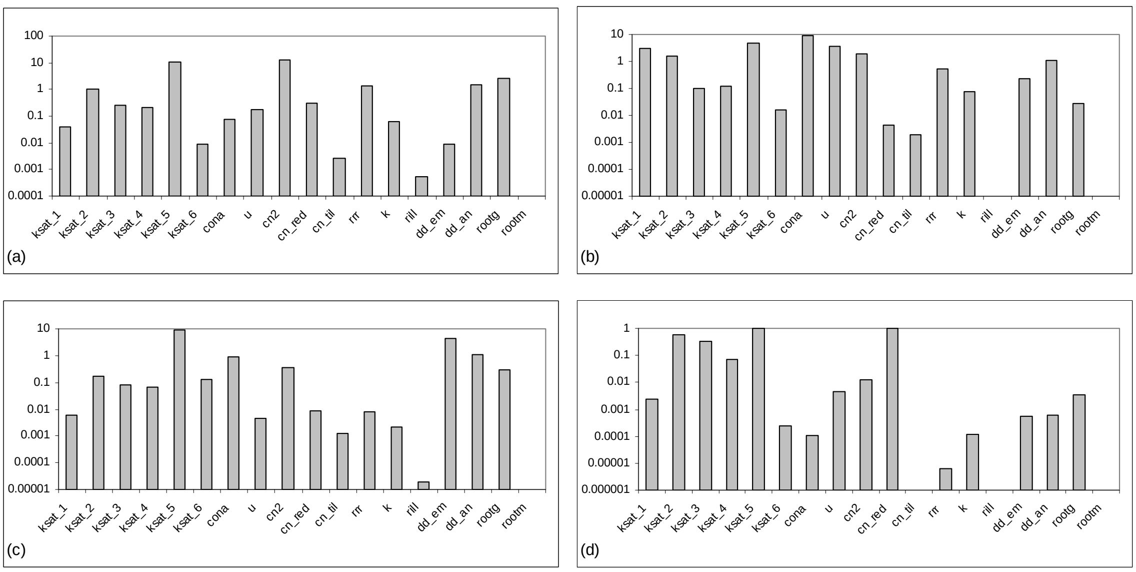

Figure 3. Parameter contributions to optimised error variance for predictions of (a) total runoff for the validation period, (b) total erosion, (c) total deep drainage, and (d) daily runoff on 13/04/1988.

The value of each type of observation data in reducing the uncertainty of the four predictions is shown in Figure 4. As would be expected, the observation data which match each type of prediction make the largest contribution to reducing its uncertainty. Of note is the large contribution that erosion data make to the runoff predictions, the relative lack of importance of other data types in predicting runoff and erosion, and the significant contribution by each data type to predicting deep drainage. These results highlight the varying importance of each data type depending on the prediction of interest.

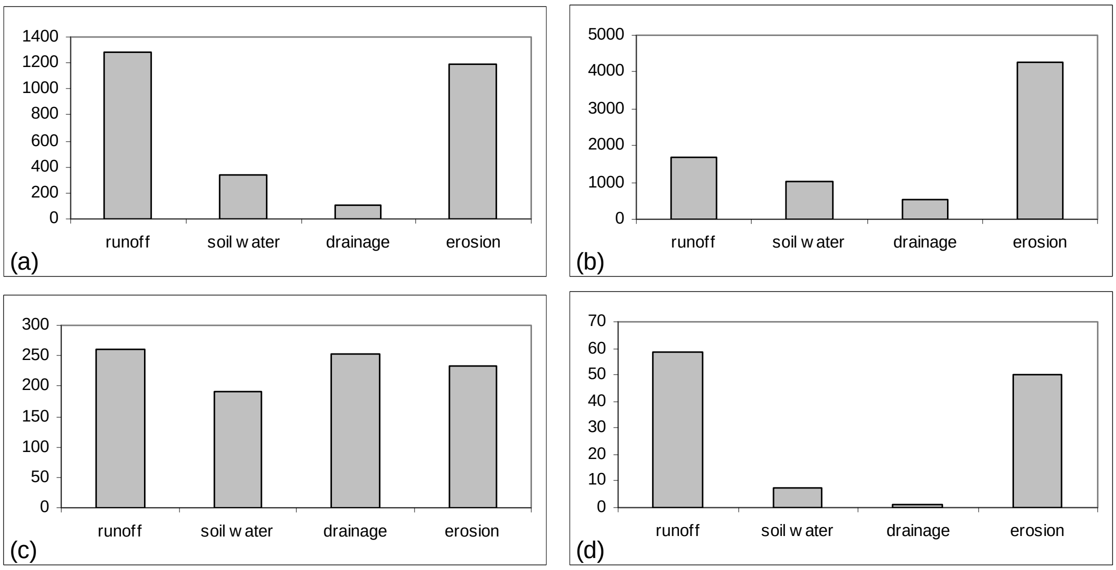

Figure 4. Decrease in error variance due to inclusion of observation data, for predictions of (a) total runoff for the validation period, (b) total erosion, (c) total deep drainage and (d) daily runoff on 13/04/1988.

4. DISCUSSION

Calculation of parameter identifiability indices showed that a large number of parameters cannot be estimated, even with the reasonably comprehensive experimental dataset that is available for the Greenmount site. This analysis was limited, however, by the use of data from only the burnt stubble treatment; it could be repeated with data from different fallow treatments and also with horizon soil water data, to confirm which parameters can be estimated and which (if any) cannot be constrained at all. This information will allow modellers to gain efficiencies, by fixing some parameters with the knowledge that calibration data are unlikely to inform their true values.

The uncertainty bounds for key predictions are as good as, or better, than expected of the model. This indicates that some sources of uncertainty may still be unaccounted for. The omission of the soil water parameters and some crop parameters from this study supports this theory. Repeating the assessment with a more comprehensive set of parameters could refine these uncertainty estimates. Uncertainty of other predictions, such as soil water contents, and predictions over different time scales, could also be explored.

In spatial applications, PEFECT is used without data for formal validation, instead there is the assumption that sensible parameter values can be identified for a range of environmental conditions which will result in predictions that are accurate at least in a relative sense. Based on the results of this study, focus can be directed to estimating parameters which have been shown to make the largest contributions to predictive uncertainty, while the remaining parameters can be fixed at default values. As shown in Figure 4, parameter contributions vary depending on the type of prediction being made. The next step toward assessing uncertainty of spatial modelling could be to repeat this study using more general assumptions for preferred parameter values and wider parameter bounds, reflecting the situation where modellers must parameterise spatial scenarios based only on extrapolation from calibrated sites and expert knowledge. This would be expected to result in much wider uncertainty bounds than those for a well studied site such as Greenmount.

This study used methods based on assumptions of model linearity; while these assumptions would not have been entirely valid the results should be considered a reasonable assessment of predictive uncertainty. Further work could be carried out using non-linear methods, such as Monte Carlo analysis, to refine the results presented here.

5. CONCLUSIONS

PEST utilities have been used to provide valuable information on predictive uncertainty in PERFECT, which was not previously available. Information on the contributions of various parameters to uncertainty will help modellers to more efficiently parameterise scenarios in spatial modelling applications. Uncertainty bounds of key predictions were as good as, or better, than expected. In carrying out these analyses a number of questions have been raised, pertinent to both site-based and spatial modelling applications, that could be addressed in future studies.

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