The Catchment Runoff Attenuation Flux Tool, a Minimum Information Requirement Nutrient Pollution Model

R. Adams[1], P.F. Quinn[2], M.J Bowes[3]

1. School of Civil Engineering and Geosciences, Newcastle University, Newcastle upon Tyne, NE1 7RU, UK.
2. School of Civil Engineering and Geosciences, Newcastle University, Newcastle upon Tyne, NE1 7RU, UK.
3 Centre for Ecology and Hydrology, Maclean Building, Crowmarsh Gifford, Wallingford, Oxfordshire, OX10 8BB, UK.

[2]Corresponding author

Abstract

A model for simulating runoff pathways and water quality fluxes has been developed using the Minimum Information Requirement (MIR) approach. The model, the Catchment Runoff Attenuation Flux Tool (CRAFT) is applicable to meso-scale catchments which focusses primarily on hydrological pathways that mobilise nutrients. Hence CRAFT can be used investigate the impact of flow pathway management intervention strategies designed to reduce the loads of nutrients into receiving watercourses. The model can help policy makers meet water quality targets and consider methods to obtain “good” ecological status.

A case study of the 414 km^2 Frome catchment, Dorset UK, has been described here as an application of the CRAFT model in order to highlight the above issues at the meso-scale. The model was primarily calibrated on ten year records of weekly data to reproduce the observed flows and nutrient (nitrate nitrogen - N - and phosphorus - P) concentrations. Data from two years with sub-daily monitoring at the same site were also analysed. These data highlighted some additional signals in the nutrient flux, particularly of soluble reactive phosphorus, which were not observable in the weekly data. This analysis has prompted the choice of using a daily timestep as the minimum information requirement to simulate the processes observed at the meso-scale including the impact of uncertainty.

A management intervention scenario was also run to demonstrate how the model can support catchment managers investigating how reducing the concentrations of N and P in the various flow pathways. This meso-scale modelling tool can help policy makers consider a range of strategies to meet the European Union (EU) water quality targets for this type of catchment.

Key words:

Hydrological Modelling, diffuse pollution, nitrate, phosphorus, land management

1. Introduction

The meso-scale is classed as catchments that vary between 10km^2 -1000km^2 (Blöschl, 1996). Uhlenbrook et al., (2004), states 'The satisfactory modelling of hydrological processes in meso-scale basins is essential for optimal protection and management of water resources at this scale'. It is therefore important that government policies on pollution abatement be implemented at this scale. The EU Water Framework Directive (WFD) (European Parliament, 2000) has required catchments to meet in-stream standards in order to obtain "Good" ecological status. Therefore, all surface water bodies must meet exacting water quality and ecological targets (Withers and Lord, 2002). There is a need for a framework that helps inform policy makers and regulators to understand the source of nutrient pollution at the scale of their interest.

Numerous models have been developed to simulate water and nutrient fluxes at the meso-scale (e.g. INCA, Wade et al., 2002, 2006; PSYCHIC, Davison et al., 2008; SWAT, Arnold, 1994). These models have been used to underpin policy decisions and feed into the decision making processes with regards to the catchment land use, and assess the impacts of any changes including source control or modified agricultural practices (Whitehead et al., 2013). However, these models tend to be too complex for informed end users to use and the simulations are prone to having greater parameter uncertainty than simpler models (McIntyre et al., 2005; Dean et al, 2009). Conversely export coefficients can be an over simplification of reality and omit the role of event driven nutrient losses (Johnes, 1996; Hanrahan et al., 2001). A series of recent catchment scale studies have investigated the role of residence time and its variability in the export of nutrients (particularly nitrate and conservative tracers (e.g. chloride); Botter et al., 2011; Hrachowitz et al., 2013;Van der Velde et al., 2010), in small catchments (<10 km^2) to identify travel time distributions. These studies focussed on small research catchments with more extensive datasets, including high-resolution DEMs. Moreover, their scope was limited firstly in terms of the number of different nutrients investigated; and secondly in the number of flow pathways; for example Van Der Velde et al. (2010) only considered a single pathway (shallow groundwater) that transported nitrate from the catchment to the stream without any representation of overland flow in their model.

High frequency (defined here as containing sub-daily data) water quality monitoring data sets are becoming increasing available with newly developed auto-analysers and sondes (for example: Cassidy and Jordan 2011; Owen et al., 2012; Wade et al., 2012), and from high frequency samplers (Evans and Johnes, 2004; Bowes et al., 2009a).

It is vital that models should aid catchment planners when considering alternative strategies to attain policy objectives (Cuttle et al., 2007; DEFRA, 2015). This study aims to show that modelling must include sufficient processes to reflect nutrient losses from the catchment which must be based primarily on soil and hillslope processes: such as overland flow; subsurface soil flow and slower groundwater dynamics (in temperate catchments). Hence the model must represent both chronic nutrient losses (seasonal fluxes), and acute losses (storm driven fluxes) (these terms were defined by Jordan et al., 2007). To this end a MIR modelling approach was developed which: (i) uses the simplest model structure that achieves the current modelling goals; (ii) that uses process-based parameters that are physically interpretable to the users so that the impact of any parameter change is clear (Quinn et al., 1999; Quinn, 2004). The CRAFT (Catchment Runoff Attenuation Flux Tool) has been developed. Hence the MIR approach leads to a parsimonious lumped model that capitalises on the mixing effects of aggregation and homogenisation of processes observed at the meso-scale.

1.1 The MIR approach

The MIR approach was developed partly as a response to a perceived excessive number of parameters in the established water quality and sediment transport models (Quinn et al., 1999; Quinn, 2004), and partly to address the issue of excessive model complexity to end user needs. In principle MIR models are based on how much information can be gained from localised and experimental studies on nutrient loss, so that the most pertinent process components can be retained in the model and be easily manipulated and assessed by an end user.

Models derived through the MIR approach must be suitable for use in the decision-making process in order to become a valuable tool. In this approach the issues that require addressing include: (i) the complexity of the model, (ii) linking nutrient losses and hydrological flow pathways and (iii) the ability to simulate both acute and chronic nutrient fluxes.

In the MIR approach, the modelling of runoff is kept as simple as possible, although key runoff processes that influence nutrient and sediment loads are retained (Quinn, 2004). By creating a meta model of more complex process based models, a minimum number of processes are retained in the model structure that are required to satisfy a model goal: in this case the simulation of meso-catchment scale diffuse pollution. A series of simple equations are implemented in MIR models with a parsimonious number of parameters. The TOPCAT MIR family of models (Quinn, 2004, Quinn et al., 2008) were developed using this approach to simulate various sources of sediments and nutrients. Heathwaite et al. (2003) developed a simple spatial index model for estimating diffuse P losses from arable lands into waterways called the PIT (Phosphorus Indicators Tool). A series of Decision Support System (DSS)-based models were developed in Australia: commencing with E2 (Argent et al., 2009), then WaterCAST and finally SourceCatchments (Storr et al., 2011; Bartley et al., 2012). These have similar features of a MIR including: a daily simulation timestep to predict sediment and nutrient concentrations (*C*); and fluxes (i.e. *C* x daily flow); containing only two flow and nutrient pathways termed "event mean" i.e. storm flow, and "dry weather" i.e. baseflow, both assigned fixed *C* values for each sediment and nutrient simulated.

It is important that models are seen as useful in terms of the decision making process and its relationship to land use through a feedback mechanism between the regulators (DEFRA, 2015) and the land owners (e.g. farmers as in Cuttle et al., 2007) or holders of discharge consents into receiving watercourses (e.g. water companies) (Whitehead et al., 2013). Modelling can highlight any potential problems such as changes in nutrient form, known as pollution swapping (Stephens and Quinton, 2009). In essence, the model shows how catchment management decisions impact nutrient concentrations and fluxes at the scale of assessment.

2 Methods

2.1 Catchment Description

The case study focusses on the 414.4 km^2 River Frome catchment (Fig. 1) which drains into Poole Harbour with its headwaters in the North Dorset Downs (Bowes et al., 2011; Marsh and Hannaford, 2008; Hanrahan et al., 2001). Nearly 50% of the catchment area is underlain by permeable Chalk bedrock, the remainder consists of sedimentary formations such as tertiary deposits along the valleys of the principal watercourses (including sand, clay and gravels). There are some areas of clay soils in the lower portion of the catchment. However, most of the soils overlaying the chalk bedrock are shallow and well drained. The land use breakdown is dominated by improved grassland (*ca*. 37%, comprising hay meadows, areas grazed by livestock and areas cut for garden turf production), and *ca*. 47% tilled (i.e. arable crops primarily cereals) usage (Hanrahan et al., 2001). The major urban area in the catchment is the town of Dorchester (2006 population over 26000, Bowes et al., 2009b) otherwise the catchment is predominantly rural in nature.

The mean annual catchment rainfall was 1020 mm and mean runoff 487 mm from 1965 to 2005 (Marsh and Hannaford, 2008). At East Stoke the UK Environment Agency (EA) has recorded flows since 1965. The Centre for Ecology and Hydrology (CEH) and Freshwater Biological Association have collected water quality samples at this same location at a weekly interval from 1965 until 2009 (Fig. 1) (Bowes et al., 2011), see 2.1.2 below.

Hanrahan et al. (2001) calculated both export coefficients for diffuse sources of TP, and load estimates for diffuse and point sources (comprising: WWTPs (serving Dorchester plus other towns); septic systems; and animal wastes). The total annual TP (total phosphorus) export from diffuse sources in the catchment was estimated to be 16.4 t P yr^{-1}, a yield of 0.4 kg P ha^{-1} yr^{-1}. Point source loads from WWTPs, septic systems and animals added an extra 11.5 t P yr^{-1} (from the data in Table 2 in Hanrahan et al. (2001)) to the catchment export, giving a total load of 27.9 t P yr^{-1}. Nitrogen (as nitrate) export from the catchment in the mid-1980s was estimated by Casey et al. (1993) to be 21.6 kg N ha^{-1} yr^{-1}, with 7% of this originating from point sources in the catchment.

2.1.1 Meteorological Data

Forcing data (precipitation) was supplied by the EA for the period 1997 to 2006 which was therefore chosen as the modelling period. A single raingauge, Kingston Maurwood (ST718912) located ca. 4 km downstream of Dorchester, was used for the modelling as this gauge had the most complete record and was centrally located in the catchment. Daily mean and 15-minute interval flow data were also provided from East Stoke gauging station for the same time period. Potential Evapotranspiration (PET) was derived using an algorithm developed to calculate a daily PET based on monthly temperature patterns, in order to obtain a daily PET time series which when totalled for the year would match the estimated annual PET (465 $mmyr^{-1}$). Given the dominance of winter runoff in the Frome catchment the model predictions are unlikely to be sensitive to input values of PET.

2.1.2 Monitoring Datasets

Two sets of water quality monitoring data were used in this study with daily flows recorded by the Environment Agency at East Stoke gauging station. The data were compared and analysed so that the MIR model could be defined. The attributes of the data are described in Table 1 and long term statistics relating to nutrient concentrations are listed in Table 2. The first is the CEH/Freshwater Biological Association long-term dataset (LTD) of water quality for the River Frome (Bowes et al., 2011; Casey, 1975; open access via gateway.ceh.ac.uk). After March 2002 the introduction of P-stripping measures at Dorchester WWTP produced a step reduction in SRP concentrations and reduced SRP loads by up to 40%, according to the analysis of Bowes et al. (2009b). The second dataset (Table 1) is a high frequency data set (HFD) described in Bowes et al. (2009a) which was also collected at East Stoke overt a shorter period using a stratified sampling approach and EPIC™ water samplers (Salford, UK). High resolution measurements may be prone to localised "noise" that can introduce errors to the observations (Bowes et al., 2009a). Unravelling trends, seasonality and "noise" may require signal processing techniques to extract meaningful time series data and perform trend analysis (e.g. Kirchner and Neal, 2013).

2.1.3 Temporal Runoff and Nutrient Behaviour in the Frome Catchment (LTD and HFD)

The flow timeseries of the LTD (daily mean flows; DMF) and HFD (sub-daily) flows were compared over the HFD monitoring period and both time series of flows are shown in Fig. 2a along with the residuals. For most of the period both sets of flows closely matched (ρ = 0.98) except perhaps during runoff events of less than a day where the HFD flows were sometimes higher as indicated by the positive residuals. The analysis suggests that, for modelling purposes including load estimation, that a daily timestep can capture the variability in the observed data without the need to use an hourly timestep.

For nitrate it is assumed that nitrite concentrations were negligible in the LTD dataset (Bowes et al., 2011) so that TON concentrations (equivalent to nitrate plus nitrite) were effectively equal to nitrate. This allows the HFD TON data to be directly compared against the observed (weekly LTD) nitrate data. The patterns observed visually (i.e. locations of the peak *Cs*) in the weekly and high frequency nitrate/TON timeseries were very similar indicating that the weekly monitoring data were probably sufficient to estimate the range of nitrate/TON concentrations in the catchment, in order to assess compliance with EU WFD quality standards (in this case ensuring that $C \leq 11.9$ mgL^{-1} N). In Fig. 2b it can be seen that there were a few spikes in the HFD above concentrations measured by the LTD, with those measured during recession spells in the flows generally being less than 1 mgL^{-1} N in magnitude. There was also no evidence that high flows would generate correspondingly high nitrate concentrations and in fact, in Fig. 2b a dilution effect can be clearly observed during several events in autumn 2005 (indicated by "1", and the dashed blue line linking the concentration timeseries to the corresponding events in the hydrograph in Fig 2a), with lower concentrations persisting in some cases for several days after the event. This indicates that concentrations of nitrate in the combined slower baseflow / sewage effluent must have been higher than concentrations in rapid overland flow.

For phosphorus the HFD SRP data were compared visually with the LTD SRP data in Fig. 2c and again the patterns in both datasets were broadly similar, with increasing concentrations during the summer period between May and November 2005. HFD TP concentrations are also shown in Fig 2c by the red line. Between November 2004 and March 2006 there was a gap in the LTD TP data for operational reasons discussed in Bowes et.al (2011). Several key points arising from the HFD data are:

(i) Some of the spikes in TP concentration, for example in February and mid-December 2005, were during the falling limb or low-flow periods of the hydrograph and were not associated with significant storm runoff events. Corresponding spikes in SRP concentration were not usually prominent at these times except for one in January 2006. (Examples are indicated by "2" on Fig. 2c). Some spikes were also observed during medium flow periods on several occasions in summer 2005, without corresponding SRP spikes but during a period where SRP concentrations were increasing. (Examples are indicated by "3" on Fig. 2c).

(ii) Three events between November 2005 and 1st January 2006 did generate high concentrations in PP that coincided with the storm peak in the flow hydrograph (>1 mg L^{-1} P). This could indicate a faster mobilisation of PP into the channel system during wet conditions in autumn-winter 2005 compared to summer storms. Haygarth et al. (2012) have observed similar peaks in PP in smaller headwater catchments due to sheet flow events. (Examples are indicated by "4" on Fig. 2c). Some smaller "Type 4" events were also observed between February and April 2005.

(iii) Some SRP concentration spikes were not simultaneously observed in the TP concentrations, these may have been due to WWTP discharges or leaky septic tanks (the high sampling frequency permitted this to be observed; Bowes et al. (2009a)). Examples of these are indicated by "5" on Fig. 2c.

SRP concentrations during the summer months tended to increase by approximately 0.07 mgL^{-1} P indicating chronic sources of nutrients in the catchment whereas acute sources tended to be associated with runoff events or other events in the catchment not associated with high flows. Bowes et al. (2011) also observed this phenomenon in the LTD dataset and suggested that the probable cause was a combination of lower flows with less dilution of SRP in the river originating from point sources (WWTPs) in the catchment. Jordan et al. (2007) attributed acute sources of TP in their 5 km^2 agricultural catchment in Northern Ireland to applications of slurry and inorganic P during periods of low rainfall (with no associated runoff events).

Of the 12 runoff events observed between February 2005 and Feb 2006, 9 were classified as "Type 4" events in terms of TP, where a corresponding increase in TP *C* was also observed (Fig 2c). The total annual loads (1/2/2005-31/1/2006) of TP and SRP were estimated from the HFD using simple baseflow separation and load analysis techniques as carried out by Haygarth et al. (2005) and Sharpley et al. (2008) in order to estimate the percentage of the annual TP load generated by events. These loads (with the % contributed from the 9 runoff events in brackets) were estimated to be 27.8 t TP (20.0 %) and 13.1 t SRP (17.7 %) respectively.

Figure 3 goes around here

The total annual TP loads are shown in Fig. 3 as a pie chart that indicates the percentages due to event and non-event sources. The percentage of the SRP load from point sources (mostly WWTPs) was estimated to be 34% based on Bowes et al. (2011) and is indicated by the dashed segment (i.e. 4.5 t P). Making the further assumption that PP = TP-SRP allowed the PP load to be estimated as well (here the "PP" load estimate will probably include a component of unreactive, organic P, so it will be an overestimate) to be 14.8 t PP (22.1 % from events).

The HFD dataset shows the range of concentrations that are seen in reality which are often missed in weekly and monthly datasets. These data also show the problem of noise and incidental events that are not correlated to storms. Hence the meso-scale model requires a structure that can address the identifiable seasonal and event driven patterns but equally should not be expected to exhibit high goodness of fit metrics.

2.2 Model Description

2.2.1 Developing the CRAFT model using the MIR approach

The justification for including some processes and omitting others is a difficult task in modelling. Hence it is worth firstly reviewing the MIR process to date. CRAFT has evolved from the model TOPCAT-NP (Quinn et al., 2008). In terms of the hydrology, TOPCAT-NP contained a dynamic store model and a constant (flow and concentration) groundwater term. TOPCAT-NP also contained a time varying soil leaching model for N and SRP (with an associated soil adsorption term for SRP).

In terms of nutrient process modelling (in TOPCAT-NP), a meta-modelling exercise of the physically based model EPIC (simulating flow, SS, N and P) (Williams, 1995) and the N-loss model SLIM (<u>S</u>olute <u>L</u>eaching <u>I</u>ntermediate <u>M</u>odel) (Addiscott and Whitmore, 1991) was carried out and are published in Quinn et al. (1999). Herein a case was made to reduce many of the soil hydrological and chemical processes. Multiple simulation of EPIC showed that both the annual exports and the daily losses could be readily simulated by a leaching function and knowledge of how much N or P was being applied and available for mobilisation. Based on these earlier studies, the final version of TOPCAT could simulate flow, N and P at a number of research locations (hence the suffix "-NP"). It included a leaching model; hence a soil nutrient store and a leaching term based on a soil type parameter were required to determine the flux into the store.

Essentially the MIR formulation is thus a series of mass balance equations that sum the flux of nutrients $F=C.Q$ from each store over time to obtain a nutrient load. In order to study nutrient pools and/or explicit soil flux processes then a physically based model is required (e.g. Arnold (1995); Van der Velde

(2010); Hrachowitz et al., 2013). The HFD dataset (Section 2.1.2) described above is used to estimate the likely origin and magnitude of nutrient fluxes in the catchment and help inform our choice of model structure in terms of processes and stores. The second simplest form of a MIR water quality model (other than merely using a constant concentration of nutrients in all the stores) is the EMC/DWC formulation (Argent et al., 2009) with two stores: (i) "Dry Weather", i.e. baseflow; (ii) "Event Mean", i.e. overland flow events in this case. Each store is represented by a single, constant *C* value, i.e. DWC and EMC respectively.

The results of modelling nitrate using a two-store MIR model can be seen in Fig 2b by the green line. The two *C* parameters are respectively 6.5 mg L^{-1} N (DWC) and 2 mg L^{-1} N (EMC). Here, the "flow" component of the MIR is able to reproduce events (here with lower nitrate *C*) reasonably well, but the background nitrate *C* is not reproduced well during the summer-autumn period since the model overpredicts it between July-November 2005. A similar phenomenon could be demonstrated using the SRP dataset with this structure of MIR model. The modelling of the Frome catchment using a CRAFT MIR will be revisited later, but this exercise neatly illustrates how an MIR model can be too simple to represent all the phenomena that are detectable in the observations. Thus TOPCAT-NP's constant (flux and *C*) groundwater term was hence too simple for this study.

The signals observed in the HFD dataset are examined slightly more deeply, in order to further develop the conceptual MIR model processes (particularly for P). Nine of the twelve events discussed above were classified as "Type 4" events in terms of TP, where a corresponding increase in the TP *C* was also observed (Fig 2c). These should be incorporated in a MIR model, if it is to be a useful predictive tool for modelling P event fluxes and TP loads, by generating TP (as PP) from runoff events. In Fig 2c it was indicated that the TP Cs during "Type 4" events were quite variable (highest in late autumn-winter 2005) so that using a constant C value in the overland flow/surface process store in a MIR model would be an oversimplification.

The Type 2 and 3 events discussed above generated spikes of relatively high TP *C*s and Type 5 events generated spikes of SRP *C*s that were not associated with significant catchment rainfall, or flow events observed at the outlet (Fig 2c). Therefore, in terms of total annual P loads the Type 2 and 3 events contributed a very small percentage of the total (mainly due to the low flows at the time of occurrence, and may have been generated by incidental losses.

In Fig 2b it was shown with the HFD TON signal that many of the runoff events were categorised as "Type 1" where dilution of the TON, presumably due to overland flow, was observed. A similar analysis to that carried out with the TP data was not appropriate as it was clear that the TON *C* in overland flow during events must have been lower than the observed *C* in the baseflow in order to have caused the dilution patterns. Thus the MIR model should capture: (i) a dilution signal; (ii) the observed variations in TON *C*s, particularly the decrease observed between later winter and summer (i.e. in the winter 2005-6 period from ca. 7 mg L^{-1} N to ca. 4 mg L^{-1} N followed by a recovery back up to 7 mg L^{-1} N). The two store MIR model shown in Fig. 2c was unable to reproduce any seasonal patterns at all in the observed TON HFD data.

Therefore, it was decided that an additional flux term (and store) was required in the model to represent a time-varying baseflow component from deeper groundwater (GW). This modification also had a similar beneficial effect on the modelling of the SRP concentrations. The shape of the flow hydrograph and some background information on the catchment physical characteristics (Casey et al., 1993; Marsh & Hannaford, 2008) suggested that an improved representation of the subsurface flow processes was important in the Frome catchment. In meso-scale catchments such as this a physically-based leaching function (as used in TOPCAT-NP; Quinn et al., 2008) thus also becomes redundant as the 'minimum requirement' is to know the concentration of the nutrients at the outlet and it is assumed that fluxes of N and P are being generated at some location in the catchment throughout the year, due to the (assumed uniform) spatial distribution of intensive agricultural land uses. These fluxes are thus incorporated into a soil flux store in the final MIR with this flux assigned constant *C*s of SRP and N.

The development of the conceptual model discussed above led to an MIR structure for the CRAFT model that represents the complex hydrological system in the simplest manner feasible. The upper pane of Fig. 4 shows that the model comprises three dynamic storages and the associated flow and transport pathways (or fluxes). The lower pane in Fig. 4 shows the flow and nutrient transport pathways that exist in a catchment such as the Frome using a conceptual cross-section of a hillslope. Here, inputs and outputs of N and P in the catchment are shown diagrammatically. There are three flow pathways shown: (i) an overland flow component which also represents processes in the cultivated near surface layer (down to several centimetres depth); (ii) a faster subsurface component encapsulating agricultural soils that may have been degraded by anthropogenic activities and perhaps enhanced flow connectivity (e.g. through field drains); (iii) a slower groundwater component encapsulating any background flow in the catchment due to: deeper flow pathways; Wastewater Treatment Plants (WWTP) discharges (assumed constant); and other non-rainfall driven constant fluxes including any generated within either the channel or the riparian areas. We will refer below to the pathways as: (i) overland flow (OF); (ii) fast subsurface soil flow (SS); and (iii) as the slow, deeper groundwater flow pathway (DG) respectively. It has been argued above that the composition of SRP and nitrate fluxes must be dominated by the DG and SS pathways. The TP flux includes a PP component that is generated by the OF pathway in the model (as discussed above).

2.2.2 Water Flow Pathways

There are six parameters that require estimation or calibration to control the water flow pathways. Their values are shown in Table 3 below.

The uppermost dynamic surface store (DSS) is conceptualized to permit both crop management and runoff connectivity options to be examined. The DSS store is split into two halves with the upper half representing a cultivation (tillage) layer that generates overland flow, and the lower half controls the ET and the drainage rate to the lower stores. Firstly, a water balance updates the storage (S_S) and then computes the overland flow from the surface store (Q_{OF}) through the following equations, where R is rainfall, D drainage to the lower half of the store. Note that all stores are in units of length (e.g. m) and all flux rates (e.g. R, D, Q_{OF}) are in units of length per time step (e.g. m .day^{-1})

$$S_S\,(t) = S_S\,(t\text{-}1) + R(t) - Q_{OF}\,(t\text{-}1) - D\,(t\text{-}1) \qquad (1)$$

$$D(t) = \mathrm{Min}\,(S_{DMAX}, S_S(t)) \qquad (2)$$

$$Q_{OF}\,(t) = (S_S\,(t) - D(t)) \cdot K_{SURF} \qquad (3)$$

The parameter S_{DMAX} can be used to deliberately partition excess water between surface and subsurface flows which is crucial for investigating connectivity options and possible pollution swapping effects. The lower half of the SCS represents the soil layer (below the cultivated layer) and also accounts for losses due to actual evapotranspiration E_T. The parameter limiting the size of the store is called S_{RZMAX}. The storage of water in the store (S_{RZ}) at each time step is updated by the following mass balance:

$$S_{RZ}\,(t) = S_{RZ}\,(t\text{-}1) + D(t) - E_T\,(t) \qquad (4)$$

Any excess water present in the store above S_{RZMAX} will form percolation (Q_{PERC}) which then cascades into the subsurface SS and DG stores. S_{RZ} is then reset to S_{RZMAX}

$$Q_{PERC}\,(t) = \mathrm{MAX}\,(0, (S_{RZ}\,(t) - S_{RZMAX})) \qquad (5)$$

Both the SS and DG stores are dynamically time varying and generate fast (Q_{SS}) and slow groundwater flows to the outlet (Q_{GW}) respectively. A dimensionless parameter K_{SPLIT} (0,1) apportions active drainage from the lower surface store towards either store, i.e. a water balance for the storage (S_{SS}) in the SS store can be written as

$$S_{SS}\,(t) = S_{SS}\,(t - 1) - Q_{SS}\,(t - 1) + Q_{PERC}(t) \cdot K_{SPLIT} \qquad (6)$$

The equation for the storage in the DG store (S_{GW}) is identical except that (1 - KS_{PLIT}) is substituted for K_{SPLIT} and S_{GW} for S_{SS}.

The flow (Q_{SUB}) from either subsurface store is described by Eq. (7) where K is a recession rate constant (d^{-1}) and S is the storage (in m). Therefore Q_{SUB} at time t, is given by

$$Q_{SUB}(t) = K\,S(t\text{-}1) \tag{7}$$

In the DG store the initial storage S_{GW0} is set by the user by rearranging Eq. (7) in terms of the groundwater discharge Q_{GW0} at the start of the simulation (assumed to be equal to the observed flow in a dry spell)

$$S_{GW0} = {Q_{GW0}}/{K_{GW}} \tag{8}$$

Where Q_{GW0} ≡ Observed runoff on first day of simulation (m d^{-1}), following the assumption above

Lastly, the total modelled runoff at each timestep, at the outlet is calculated (Q_{MOD})

$$Q_{MOD} = Q_{OF} + Q_{SS} + Q_{GW} \tag{9}$$

2.2.3 Nutrient Fluxes

The user must now add a sensible range of input nutrient concentrations to the model in order to simulate loads (i.e. *C x Q*). They are encouraged to set and alter these values and see the impact instantaneously. The nutrient transport processes are conservative and the user is encouraged to understand the link between land use management and the level of nutrient loading assuming that they have a working knowledge of the relevant terms and processes.

In general nutrients are modelled in the CRAFT by either a constant concentration assigned to each flow pathway or by using an uptake factor (or "rating curve") approach (e.g. Cassidy and Jordan (2011); Krueger et al., (2009)), where the concentration is directly proportional to the overland flow rate (Eq. (10)). A conceptual model of the flow and transport pathways in the catchment that are incorporated in the CRAFT is shown in the lower part of Fig. 4.

In the uptake factor approach, the concentration vector (units mg L^{-1}) of different nutrients (**n**) in overland flow (C_{OF}) is given by

$$C_{OF}(\mathbf{n}) = \mathrm{MAX}\,(K(\mathbf{n}) \cdot Q_{OF},\ C_{OFMIN}(\mathbf{n})) \tag{10}$$

Where: Q_{OF} is the overland flow; $K(\mathbf{n})$ represents the slope of the relationship between flow and nutrient (**n**) concentration in the observed data (i.e. uptake factor) and $C_{OFMIN}(\mathbf{n})$ is the minimum concentration. This is included in Eq. (10) to prevent unrealistically low concentrations being used in the model during low flow periods, i.e. below the measurable limit. Krueger et al. (2009) used this type of equation to model TP concentrations in high flows generated by enrichment of sediment with P.

The daily nutrient load is calculated by the mixing model described by Eq. (11), where L(**n**) is the vector of the nutrient loads (NO_3, SRP and TP, denoted by **n**), C_{SS} and C_{GW} are the constant concentrations in the dynamic soil and dynamic groundwater zones respectively

$$\mathrm{L}(\mathbf{n}) = C_{OF}(\mathbf{n}) \cdot Q_{OF} + C_{SS}(\mathbf{n}) \cdot Q_{SS} + C_{GW}(\mathbf{n}) \cdot Q_{GW} \tag{11}$$

The concentration vector of the nutrients in the catchment outflow ($C(\mathbf{n})$) can be calculated directly from the vector $L(\mathbf{n})$ using Eq. (12)

$$C(\mathbf{n}) = L(\mathbf{n}) / Q_{MOD} \tag{12}$$

Nitrate and SRP concentrations are calculated at each timestep using Eqs. (11) and (12). The TP concentration is calculated by Eq. (13)

$$C(\mathrm{TP}) = \frac{L(\mathrm{SRP}) + L(\mathrm{PP})}{Q_{MOD}} \tag{13}$$

CRAFT can thus capture the mixing effects of N and P losses associated with several hydrological flow pathways at the meso-scale. The above equations that remain in the MIR for CRAFT do not contain:-

i) The myriad of nutrient cycling processes occurring in the N and P cycles. Section 2.1.2 shows the observable processes at the catchment outlet and Figure 3 the nutrient apportionment at this scale. However, the MIR captures the integrated effect of the processes and how these might change over time.

ii) Riparian processes are not explicitly included in the model. However, it is argued the impact of these processes is not observable at the outlet. The net effect of riparian processes are integrated into the soil and groundwater concentration values.

iii) Within channel processes such as plant uptake and the bioavailability of nutrient from bed sediments. Again, the impacts of these processes are not identifiable in the HFD time series. Unless the evidence of impact is clear they are not included in the MIR process.

2.3 Modelling and Calibration

Flow and nutrients were simulated with the CRAFT for a ten year baseline period, 1 January 1997 to 31 December 2006 using a daily timestep. A comparison of the model performance at predicting the SRP and TP concentrations was curtailed at the end of February 2002. However, for nitrate the model performance over the full 10 yr period was assessed.

The performance of the calibrated CRAFT model at reproducing observed stream flow at the catchment outlet was assessed by a combination of visual inspection of the modelled against observed runoff and the use of the Nash-Sutcliffe Efficiency (NSE) evaluation metric. The hydrological model calibration aimed originally to maximise the value of the NSE whilst ensuring that the MBE (mass balance error) was less than 10%. The parameters K_{SURF}, K_{GW}, K_{SS}, K_{SPLIT}, S_{RMAX} and S_{DMAX} were adjusted iteratively to enable this and obtain a single "expert" parameter set for the baseline simulation (values shown in Table 3). The calibration strategy involved firstly obtaining an acceptable simulation of overland flow. In order of process representation: $\mathrm{K_{SURF}}$ and $\mathrm{S_{DMAX}}$ control the generation of overland flow (S_{DMAX} must be adjusted to less than the maximum rainfall rate to initiate overland flow, and then K_{SURF} controls the flow volume); K_{SPLIT} is then used to proportion recharge to the two subsurface stores; S_{RMAX} controls the timing and volume of recharge events; and finally K_{GW} and K_{SS} are adjusted to reproduce the observed recession curves in the hydrographs (K_{SS} being the more sensitive of the two).The sensitivity of the model was then assessed by running a Monte Carlo analysis of 100000 simulations, where the six parameters were randomly sampled from a uniform distribution (the upper and lower bounds are shown in Table 3).

Simulations with a MBE greater than 10% were rejected. The top 1% of simulations meeting both criteria were thus chosen as "behavioural" and a normalised likelihood function ($L(Q)_\mathrm{i}$) was calculated using Eq. (14) with the SSE values determined above for each simulation i.

$$L(Q)_i = \mathrm{SSE_i} \Big/ \sum \mathrm{SSE} \tag{14}$$

Lastly, weights were assigned to the behavioural flows based on the likelihood of each simulation. These weighted flows were then used to compute the upper and lower bounds (here the 5th and 95th percentile flows were chosen) applied to the modelled flows (Q_{MOD}).

The NSE metric is suitable for assessing flow simulation performance but is less suitable for nutrient concentrations due to the occurrence of negative NSE values, partly as a result of calculating variance terms using sparse observed data (where the sample mean is unlikely to reflect the true mean). Therefore, the nutrient model parameters were calibrated by assessing the performance of the model against the weekly concentration data in the LTD, using the following metrics to determine an "expert" parameter set:

- Visually comparing the time series of nitrate, SRP and TP against the observed data and adjusting the nutrient model parameters to obtain a best fit between modelled and observed time series.

- Optimising the errors between modelled and observed mean and 90th percentile concentrations with the aim of reducing these below 10% if possible. The mean and 90th percentile concentrations were chosen as these represent the concentrations over the range of flows (mean) and events (90th percentile), and therefore allow the model performance under all flow regimes to be assessed.

A further sensitivity analysis was then performed using the flows from the behavioural hydrology simulations (discussed above) and re-running the nutrient model (without adjusting the "expert" parameter values for the nutrients) to determine a set of upper and lower bounds (5th and 95th percentile values) to the predicted concentrations and their associated loads ($Q \cdot C$).

2.4 Management Intervention Scenario

For a model to be effective at the management level it needs to be to demonstrate the impacts of changes in local scale in land management. Here the local land use change is assumed to occur at all locations. Nevertheless, the CRAFT model can show the magnitude and proportion of the nutrients lost by each hydrological flow pathway. Equally it is possible to show the concentration of each nutrient at each time step as this helps educate the end user.

In order to demonstrate the impact of a catchment management intervention strategy, the following changes were made to the catchment as a runoff and nutrient management intervention (MI) scenario. For simplicity a combination of land use changes were applied and the output expressed as the changes in export loads for each pathway at the outlet, shown below:

(i) The modelled overland flow was reduced by reducing the value of the K_{SURF} parameter to 0.012, representing a management intervention that removes or disconnects the agricultural pollution "hotspots".

(ii) Nutrient loads in the rapid subsurface zone were reduced by reducing the values of C_{SS}(SRP) and C_{SS}(NO_3) by 50% (i.e. halving the impact of diffuse sources linked to the outlet by this flow pathway) to represent improved land management with reduced fertilizer loads. No change to the DG nitrate concentration was made as firstly, any changes in land management may take decades to be observed in the deeper groundwater (Smith et al., 2010); and secondly, recent improvements to WWTPs have only targeted reducing SRP loads and not nitrate loads (Bowes et al, 2009b, 2011).

(iii) Background loads of SRP in the catchment are reduced by lowering C_{GW}(SRP) to represent the reduction in deeper groundwater concentration caused by both lower leaching rates from the soil store and making further improvements to WWTPs in the catchment to reduce SRP loads. Bowes et al. (2009b) found that a 52% reduction in the SRP export from point sources had taken place since 2001 in the catchment (up to 70% of the SRP loads from each improved WWTP is assumed to be stripped out). In terms of the total (point and diffuse) SRP load, Bowes et al. (2011) estimated that between 2000 and mid 2009 it had been reduced by 58%, which was due to further improvements to the smaller WWTPs in the catchment as well as a reduction in diffuse sources of up to 0.1 kg P $ha^{-1}yr^{-1}$. Figure 3 shows that point sources (in 2005-6) were thus estimated to contribute 16% of the annual TP load.

3 Results

The baseline model results are shown in Fig. 5 as time series plots of modelled and observed flow at East Stoke along with the modelled and observed nitrate, TP and SRP concentrations for a selected two year period. The years chosen have average followed by wet hydrological conditions. To further illustrate the model performance at predicting flow and concentrations, the upper panes in Fig. 5 show a corresponding timeseries plot of the absolute error (i.e. Observed flow or concentration – Modelled flow or concentration).

3.1 Baseline Simulation

The hydrology model parameters used by the baseline simulation are shown in Table 3. The model results from the CRAFT were as follows: The NSE for the baseline hydrology simulation was 0.80; the mass balance error was over predicted by 1.0%. In the Frome catchment the percentage of overland flow (which includes surface runoff and near-surface runoff through the ploughed layer) according to the calibrated model was very small (2.2 % of the annual total runoff of 516 mm yr^{-1}). This value may be low but as stressed before it is difficult to see the overland flow signal at the meso-scale. Here, an overland flow component has been retained (by setting K_{SURF} and K_{SR} to the values shown in Tables 3 and 4) due to an assumption that P is being lost via this process i.e. from the knowledge arising from research studies (e.g. Owen et al., 2012; Bowes et al. 2009a; Heathwaite et al., 2005). Values for the parameters K_{SR}(PP) and K_{SR}(SRP) were determined in the baseline simulation based on some events (as suggested in figure 2 and 3) where runoff driven TP spikes were observed.

3.2 Runoff

It is possible to optimise the parameter values in the model to generate either a smaller mass balance error or a larger value of the NSE metric (over 0.8 is possible with this model and data, as evidenced by the Monte Carlo simulation results). Here a compromise was sought between both these metrics, retaining the overland flow process (discussed above) and a good visual fit with the observed flows.

The behavioural flows from the Monte Carlo simulation are shown in Fig. 6 as dotted lines representing the upper (95th percentile) and lower (5th percentiles) prediction bounds. There were 511 simulations classed as “behavioural”. The envelope of the predicted flows indicates that most of the observed flows during the ten year period of data could be reproduced, supporting the choice of runoff processes represented in the CRAFT for this particular catchment. Some events may have been either missed or over predicted which could be due to limitations with using a single rain gauge in the forcing data for the model. Table 6 shows the minimum, median and maximum flows extracted from these timeseries. The table shows that the model outputs are sensitive to the parameter values.

3.3 Nutrients

3.3.1 Nitrate

The observed nitrate concentrations in Fig. 2b indicated that concentrations of nitrate in overland flow are much smaller than concentrations in baseflow, and the model parameter $C_{OFMIN}(NO_3)$ (see Eq. 10) was set to 0.4 mgL^{-1} N (Table 4). *In the baseline scenario* the proportion of nitrate loads generated by overland flow was thus fairly negligible (<1%) and the nitrate loads were split fairly evenly between the SS and DG pathways according to the model. The load from the DG contributed around 31% of the total load, compared to 43% of the modelled runoff originating from this pathway. This implies that a significant proportion of nitrate drains from the shallow subsurface (SS) immediately after storm events, probably through either enhanced connectivity due to agricultural drains or recharge into the underlying chalk aquifer (Bowes et al., 2005). The DG component includes nitrate loads from the WWTPs in the catchment which were estimated to contribute around 7% (1.5 kg N ha^{-1} yr^{-1}) of the total load based on monitoring data from the mid-1980s (Casey et al., 1993), and 14% of the modelled DG load.

Overall, the CRAFT model reproduced a moving average of the observed nitrate LTD concentrations reasonably well and mean concentrations were within 10% of the observed (Table 5). The fit between modelled and observed nitrate in terms of absolute errors (Fig. 5b upper pane) was not so good due to timing errors in predicting the onset of dilution, although visually (Fig. 5b lower pane) the model appeared to simulate the seasonal patterns of nitrate fairly well. Table 6 shows the uncertainty in nitrate loss arising from the hydrological model in terms of the 5th, 95th percentiles and medians of modelled concentrations and yields

3.3.2 Phosphorus

Bowes et al. (2009b) estimated that between 1991 and 2003, SRP provided 65% of the TP load in the Frome catchment. In the *baseline scenario*, the DG component in the model generated almost four times the load of SRP than the SS component (Fig. 7). This seems plausible as the DG component also included the SRP loads from the WWTPs, in addition to the SRP originating from springs and seeps from shallow groundwater. Again, the K_{SPLIT} parameter in the flow model had a large influence on SRP loads, by adjusting the ratio between the SS and DG components of these. The model errors, identifiable from the panels above the timeseries plots (Fig. 5) may have been caused by timing issues leading to periods of overprediction and underprediction of SRP concentrations. Visually, the SRP concentrations showed a close match, and the seasonal patterns and trends were simulated (Fig 5c). Any spikes in the observed data which were not reproduced by the model appear not to have been caused by actual hydrological runoff events (as seen in Fig. 2 and discussed above). Modelled concentrations (on sample days only) were within 10% of the observed SRP concentrations for both the mean and 90th percentile values but underpredicted the mean and 90th percentile TP concentrations by around 50% (Table 5). This may be due to additional source(s) of P not being accounted for in the model (e.g. within-channel river dynamics and/or conversion of SRP to entrained particulate forms of P as suggested by Bowes et al. (2009a)). Table 6 shows the uncertainty in the TP and SRP losses arising from the hydrological model in terms of the 5th, 95th percentiles and medians of modelled concentrations and yields.

These results however showed that high concentrations of TP associated with the transport of PP during runoff events were predicted by the Monte-Carlo and expert simulations (over 1.9 mg L^{-1} P), which was similar to the “Type 2” events identified in the HFD dataset where TP concentrations reached 1.75 mg L^{-1} P in late 2005. The LTD dataset did not contain many spikes of this magnitude in the TP concentrations, however the HFD data did measure occasional high concentrations of TP associated with runoff events (e.g. those indicated by a “4” on Fig. 2c). Figure 2c, and the model results in Fig. 5, show that the issue of fitting TP at the meso-scale is problematical and is unlikely to be improved by having a more complex model

In the baseline scenario the modelled proportion of TP (i.e. PP) generated by overland flow was about 11% which is quite high considering that only 1.2% of the modelled runoff is generated via this pathway. The PP concentrations generated by the model were calibrated by adjusting the value of the K_{SR}(PP) parameter (Table 4).

The export yields (load per unit area) for each nutrient to show the impact of the flow pathways at transporting nutrients were also calculated (see Fig. 7 and Table 6). This aggregation lends itself to comparisons with previous studies. The baseline simulation predicted a TP export of 0.69 kg P $ha^{-1}yr^{-1}$ which is slightly more than both the export rate estimated by Hanrahan et.al (2001) for diffuse and point sources in the catchment of 0.62 kg P $ha^{-1}yr^{-1}$ (for calendar year 1998). SRP loads were modelled by Bowes et al. (2009b) and the SRP export was predicted to be 0.44 kg P $ha^{-1}yr^{-1}$ between 1996-2000 (of which WWTP discharges accounted for 49%), compared to the CRAFT modelled baseline SRP export of 0.62 kg P $ha^{-1}yr^{-1}$ (between 1997 and February 2002). Similar historical estimates for nitrate export were not available, to compare with the model estimate of 32.8 kg N $ha^{-1}yr^{-1}$ over the period 1996-2005, except a single year from the HFD dataset where the TON export was estimated to be 20.2 kg N $ha^{-1}yr^{-1}$ (Bowes et al. (2009a)). Table 6 shows the uncertainty in terms of the 5th, 95th percentiles and medians of modelled concentrations and yields.

3.4 Management Intervention (MI) Scenario

The yields of nitrate and TP are summarised by the use of bar charts in Fig. 7 which illustrate the fluxes under the baseline conditions (left bars) and the MI scenario (right bar), and the relative contribution of each of the three flow pathways to these, which provides valuable source apportionment information for policy makers.

The results show that the amount of PP generated by the overland flow pathway (denoted by the blue rectangle in the baseline scenario bar in Fig. 7) has reduced to almost zero due to the reduction in overland flow, and the difference between TP and SRP export is negligible as a result. This indicates that a limited amount of "pollution swapping" is predicted so that the proportions of PP and SRP comprising TP have changed from 8.8% and 92.2% to 0% and 100% respectively under the MI scenario. Nitrate and TP loads are predicted to decrease by 34.4% and 65.0% respectively. Under the MI scenario, the nitrate concentration in the DG flow component (which includes point sources) was not reduced (it was assumed that WWTP improvements targeted P and not N). Both nitrate and SRP loads in overland flow were negligible (< 0.1%) under the baseline scenario and have been reduced to effectively zero by drastically reducing the amount of overland flow generated. SRP loads due to point sources are included in the DG component, the predicted load from this component reduced by 63%. The export of SRP via the faster SS component also reduced by 55% (to 0.045 kg P $ha^{-1}yr^{-1}$) under the MI scenario. These reductions in the SRP loads from different components compare well to the overall reductions since the 1990s in point and diffuse sources in the catchment (Bowes et al., 2009b, 2011).

4 Discussion and Conclusions

This paper has explored the role of MIR modelling methods at the meso-scale. Specifically, it has explored the information content of flow and nutrient data within a case study, that helps justify the choice of model structure and timestep. The MIR approach to modelling is thus the minimal parametric representation to model phenomena at the meso-scale as a means to aid catchment planning/decision making at that scale. The approach is based on observations made in research studies in the Frome catchment. The MIR model that was developed, CRAFT, thus focussed on key hydrological flow pathways which are observed at the hillslope scale. The nutrient components were kept very simple neglecting all nutrient cycling aspects. The CRAFT model deliberately avoids a spatial representation of local land use in this particular case study. This implies that the lumping process is appropriate for circumstances where the local variability is lost when aggregated. The model can be used in a semi-distributed form if the land use patterns justify such a new model structure and this form may help to identify the sources of the fluxes in the overall model for some applications. Future developments of the CRAFT will also permit the investigation of many features such as riparian fluxes and also the impact of attenuation on sediments and nutrient fluxes when routed through ponds and wetlands.

High frequency data (such as the HFD) for all nutrient parameters is desirable at all locations if it were affordable. However, it is shown here that at the meso-scale these data tend to reflect the “noise”, incidental losses and within-channel diurnal cycling in the system that have a limited effect on the overall signal and loads. For the Frome case study a daily timestep in the CRAFT model could simulate the dominant seasonal and storm driven nutrient flux patterns and thus aid the policy maker in considering a variety of policy decisions. It is stressed that collecting the longest possible high frequency dataset particularly for all forms of nutrients is still of the utmost importance for effective water quality monitoring and identifying the full range of observed concentrations including incidental losses (see Fig 2c). There may be some evidence here that collecting higher resolution data for nutrients helps to explain the distribution values and addresses the issues of “noise” and diurnal variability (e.g. the fluctuations in P concentrations observed in the River Enborne by Wade et al., 2012 and Halliday et al., 2014) in the datasets. Even so, it may still be beneficial to aggregate sub-daily data to daily data as a means to optimise the capabilities of a process based model, such as the CRAFT, and make use of all the relevant information actually contained in high frequency monitoring data.

The Frome case study revealed a number of interesting factors, leading to the exploration of a management intervention (MI) scenario. The mean annual SRP concentration that has to be attained in order to comply with the WFD standards for P is 0.06 mgL^{-1} P, which was achieved by the MI scenario (modelled mean = 0.053 mgL^{-1} P) by reducing the SRP concentrations in the model’s flow pathways to reduce the modelled SRP load by 61.7%. There are no explicitly defined guidelines for nitrate, except that the maximum concentration must not exceed 11.9 mgL^{-1} N, which is imposed on all surface waters in the EU under the terms of the 1991 Nitrates Directive. In terms of nitrate management in the Frome catchment, the observed data from 1997 to 2006 indicated that concentrations (at least in surface water) were below the limit without any reductions due to nutrient and/or runoff management. The CRAFT model was able to reproduce the seasonality in the observed nitrate concentrations and also make predictions of the likely reductions in concentrations and yields, due to improved management of diffuse sources in the catchment. This MI scenario reduced mean concentrations from 6 mgL^{-1} N to 4.3 mgL^{-1} N at the outlet of the Frome. Recent studies of long term trends (Smith et al., 2010; Bowes et al., 2011) showed that nitrate concentrations were observed to be rising in the Frome since the 1940s, however over the simulation period the rate of increase has slowed down and the CRAFT model could predict the weekly time series reasonably well as a result. The MI scenario shows that interventions to reduce concentrations of nitrate in rapid subsurface flow can have a significant impact at reducing the total nitrate load by 34% although this may occur at the expense of pollution swapping leading to increased nitrate fluxes to deep groundwater. Interventions to reduce the concentration of nitrate in flows originating from deeper groundwater were not investigated as these improvements could take decades to be observable at the monitoring point at the catchment outlet (Smith et al, 2010).

The results of this case study may best be viewed as event driven export coefficients when the origin of the nutrient is tied to the pathway that generated it. This informs the user as to the aggregate effect of local policy changes and the importance of storm size and frequency. Whilst we have shown that those impacts are still uncertain it could perhaps encourage more intervention in order to guarantee the success of new policy (Cuttle et al., 2007). Equally, locally observed environmental problems caused by high nutrient concentrations may well be lost due to mixing effect at the meso-scale (i.e. catchment outlet).

The CRAFT model has been shown to fit the dominant seasonal and event driven phenomena. The benefits of using the CRAFT are thus firstly that it is a useful tool which conveys the mixed effect of land use and hydrological process at the meso-scale for policy makers. The modelling process assumes that the policy maker or informed end user will then manipulate the model to see the likely impacts of regulations. The burden is still on the user to translate policy into the likely local impact, for example: reduction in N and P loading; more efficient use of N and P in soils and the acute loss of P from well-connected flow pathways. Once the parameters are changed, the net effect at the meso-scale can then be seen instantaneously. The user is encouraged to try many scenarios and to explore the parameter space. Secondly, its interactive graphical user interface that allows an instantaneous view of the changes made to the model parameters, which in itself is informative. The range of the fluxes seen can inform the user about the uncertainty of the model when making decisions and can alert them to unexpected outcomes such as pollution swapping.

The sensitivity and uncertainty analysis carried out on the hydrological model showed the impact on the resultant nutrient fluxes. The CRAFT model is intended to be just one of many required for setting policy at the meso-scale. Equally, despite the uncertainty in the model, the outputs should encourage the user in that a range of local scale polices can have a large impact on the final nutrient flux at the meso-scale. When used with other model tools and observed data the CRAFT meso-scale model can play a key role in evaluating land use change and the need to conform to WFD targets.

4 Nomenclature

CEH Centre for Ecology and Hydrology

CRAFT Catchment Runoff Attenuation Flux Tool

DTC Demonstration Test Catchments

DWC Dry Weather Concentration (i.e. in baseflow)

EMC Event Mean Concentration (i.e. in overland flow)

HFD High Frequency data set of nitrogen and phosphorus, recorded several times per day in the River Frome.

LTD Long term data set of weekly nitrogen and phosphorus measurements also in the River Frome, modelled by the baseline scenario.

MBE Mass balance error

MIR Minimum Information Required

n Vector of nutrients simulated by the model (e.g. N and P).

NSE Nash – Sutcliffe Efficiency (model performance metric)

PP Particulate phosphorus (i.e. the insoluble fraction)

SRP Soluble reactive phosphorus (from samples filtered using 0.45 µm paper)

TON Total oxidised nitrogen (nitrate + nitrite).

TP Total phosphorus (soluble + insoluble forms)

WFD Water Framework Directive

WWTP Wastewater Treatment Plant (Sewage Treatment Works)

5 Acknowledgements

The collection of both the long term and high frequency nutrient datasets was funded by the Natural Environment Research Council.

6 References

Addiscott, T.M., Whitmore A.P.: Simulation of solute leaching in soils with different permeabilities. Soil Use and Management 7: 94–102 1991.

Argent, R.M., Perraud, J-M., Rahman, J.M., Grayson, R.B., and Podger, G.M.: A new approach to water quality modelling and environmental decision support systems. Env. Model. Software. 24:809-818, 2009.

Arnold, J. G.: SWAT (Soil and Water Assessment Tool). Grassland, Soil and Water Research Laboratory, USDA, Agricultural Research Service, Temple, TX. (USA). 1994.

Bartley, R., Speirs, W.J., Ellis T.W., and Waters, D.K.: A review of sediment and nutrient concentration data from Australia for use in catchment water quality models. Marine pollution bulletin 65(4):101-116, 2012.

Beven, K.: Environmental modelling: an uncertain future?: An introduction to techniques for uncertainty estimation in environmental prediction. Routledge, Abingdon, Oxon (UK). 2009.

Blöschl, G.: Scale and scaling in hydrology. Wiener Mitteilungen, Wasser-Abwasser-Gewässer, 132, TU Wien, Wein, (Österreich). 1996.

Botter, G., Bertuzzo, E., and Rinaldo, A.: Catchment residence and travel time distributions: the master equation, Geophys. Res.Lett., 38, L11403, doi:10.1029/2011GL047666, 2011.

Bowes, M.J., Leach, D.V., and House, W.A.: Seasonal nutrient dynamics in a chalk stream: the River Frome, Dorset, UK. Sci. Tot. Env., 336(1-3): 225-241, 2005.

Bowes, M.J., Smith, J.T., and Neal, C.: The value of high-resolution nutrient monitoring: A case study of the River Frome, Dorset, UK. J. Hydrol., 378(1-2): 82-96, 2009a.

Bowes, M.J., Smith, J.T., Jarvie, H.P., Neal, C., and Barden, R.: Changes in point and diffuse source phosphorus inputs to the River Frome (Dorset, UK) from 1966 to 2006. Sci. Tot. Env, 407(6): 1954-1966, 2009b.

Bowes, M.J., Smith, J.T, Neal, C., Leach, D.V., Scarlett, P.M., Wickham, H.D, Harman, S.A., Armstrong, L.K., Davy-Bowker, J., Haft, M., and Davies, H.N.: Changes in water quality of the River Frome (UK) from 1965 to 2009: Is phosphorus mitigation finally working? Sci. Tot. Env, 409(18): 3418-3430, 2011.

Casey, H.: Variation in chemical composition of River Frome, England, from 1965 to 1972. Freshwater Biol., 5(6): 507-514, 1975.

Casey, H., Clarke, R.T., and Smith, S.M.: Increases in nitrate concentrations in the River Frome (Dorset) catchment related to changes in land use, fertiliser applications and sewage input. Chem. Ecol., 8: 105-117, 1993.

Cassidy, R. and Jordan, P.: Limitations of instantaneous water quality sampling in surface-water catchments: Comparison with near-continuous phosphorus time-series data. J. Hydrol., 405: 182-193, 2011.

Cuttle, S. P., Macleod C. J. A., Chadwick, D. R., Scholefield, D., Haygarth, P. M., Newell-Price, P., Harris, D.,. Shepherd, M. A., Chambers, B. J., and Humphrey R.: An inventory of methods to control diffuse water pollution from agriculture (DWPA). User Manual (DEFRA Project ES0203), UK, 113pp, 2007.

Davison, P.S, Withers, P.J.A., Lord, E.I., Betson, M.J. and Strömqvist, J.: PSYCHIC - A process-based model of phosphorus and sediment mobilisation and delivery within agricultural catchments. Part 1: Model description and parameterisation. J. Hyd. 350: 290-302, 2008.

Dean, S., Freer, J., Beven, K., Wade, A.J., and Butterfield, D.: Uncertainty assessment of a process-based integrated catchment model of phosphorus Stoch. Environ. Res. Risk. Assess. 23:991-1010, 2009.

Defra, Catchment Based Approach: Improving the Quality of our Water Environment https://www.gov.uk/government/uploads/system/uploads/attachment_data/file/204231/pb13934-water-environment-catchment-based-approach.pdf, 2015.

European Parliament: Common Implementation strategy for the water framework directive (2000/60/EC). Guidance document no. 5. Transitional and coastal waters: typology, reference conditions and classification systems. Brussels (Belgium), 2000.

Evans D.J., and Johnes P.: Physico-chemical controls on phosphorus cycling in two lowland streams. Part 1 - the water column. Science of the Total Environment; 329: 145-163, 2004.

Halliday S., Skeffington R, Bowes M, Gozzard E, Newman J, Loewenthal M, Palmer-Felgate, E. J., Jarvie, H. P., and Wade A. J.: The Water Quality of the River Enborne, UK: Observations from High-Frequency Monitoring in a Rural, Lowland River System. Water; 6: 150-180, 2014.

Hanrahan, G., Gledhill, M., House, W.A., and Worsfold, P.J.: Phosphorus loading in the Frome Catchment, UK: Seasonal Refinement of the coefficient modelling approach, J. Env. Qual. 30(5), 1738-1746, 2001.

Haygarth, P.M., Wood, F.L., Heathwaite, A.L., and Butler, P.J.: Phosphorus dynamics observed through increasing scales in a nested headwater-to-river channel study. Sci. Tot. Env, 344: 83-106, 2005.

Haygarth, P. M., Page, T. J. C., Beven, K. J., Freer, J., Joynes, A., Butler, P., and Owens, P. N: Scaling up the phosphorus signal from soil hillslopes to headwater catchments. Freshwater Biology, 57(s1), 7-25, 2012.

Heathwaite, A. L., Fraser, A. I., Johnes, P. J., Hutchins, M., Lord, E., and Butterfield, D. : The phosphorus indicators tool: A simple model of diffuse P loss from agricultural land to water. Soil Use and Management, 19(1):1-11, 2003.

Heathwaite, A.L., Quinn, P.F., and Hewett, C.J.M.: Modelling and managing critical source areas of diffuse pollution from agricultural land using flow connectivity simulation. J. Hydrol., 304: 446-461, 2005.

Hrachowitz, M., Savenije, H., Bogaard, T.A., Tetzlaff, D., and Soulsby, C.: What can flux tracking teach us about water age distribution patterns and their temporal dynamics? Hydrol. Earth Syst. Sci., 17, 533-564,2013. doi:10.5194/hess-17-533-2013.

Johnes, P.J.: Evaluation and management of the impact of land use change on the nitrogen and phosphorus load delivered to surface waters: the export coefficient modelling approach, J.Hydrol. 183(3):323-349, 1996.

Jordan, P., Arnscheidt, A., McGrogan, H., and McCormick, S.: Characterising phosphorus transfers in rural catchments using a continuous bank-side analyser. Hydrol. Earth Syst. Sci., 11(2): 372-381, 2007. doi:10.5194/hess-11-372-2007

Kirchner, J.W., and Neal, C.: Universal fractal scaling in stream chemistry and its implications for solute transport and water quality trend detection, PNAS, 110, 12213-12218, 2013.

Krueger, T., Quinton, J. N., Freer, J., Macleod, C. J., Bilotta, G. S., Brazier, R. E., Butler, P., and Haygarth, P. M.: Uncertainties in data and models to describe event dynamics of agricultural sediment and phosphorus transfer. Journal of Environmental Quality, 38(3), 1137-1148, 2009.

Marsh, T. J. and Hannaford, J. (Eds.): UK Hydrometric Register, Hydrological data UK series, Centre for Ecology and Hydrology, Wallingford (UK), 210 pp., 2008

McIntyre, N, Jackson, B, Wade, AJ, Butterfield, D. and Wheater, H.S.: Sensitivity analysis of a catchment-scale nitrogen model. J. Hydrol. 315(1-4):71-92, 2005.

Owen, G. J., Perks, M. T., Benskin, C. M. H., Wilkinson, M. E., Jonczyk, J., and Quinn, P. F.: Monitoring agricultural diffuse pollution through a dense monitoring network in the River Eden Demonstration Test Catchment, Cumbria, UK. Area, 44(4), 443-453, 2012.

Quinn, P.F., Anthony, S. and Lord E.: Basin scale nitrate modelling using a minimum information requirement approach. In Water Quality: Processes and Policy, Trudgill S. Walling D, Webb B (eds). Wiley: Chichester, UK; 101-117, 1999.

Quinn, P.: Scale appropriate modelling: representing cause and effect relationships in nitrate pollution at the catchment scale for the purpose of catchment scale planning. J. Hydrol. 291: 197-217, 2004.

Quinn, P., Hewitt, C.J.M. and Dayawansa, N.D.K.: TOPCAT-NP: a minimum information requirement model for simulation of flow and nutrient transport from agricultural systems, Hydrol. Process. 22(14):2565-2580, 2008.

Sharpley, A.N., Kleinman, P.J.A., Heathwaite, A.L., Gburek, W.J., Folmar, G.J., Schmidt, J.P.: Phosphorus loss from an agricultural watershed as a function of storm size. J. Environ. Qual. 37, 362 – 368. http://dx.doi.org/10.2134/jeq2007.0366. 2008

.Smith, J.T., Clarke, R.T. and Bowes, M.J.: Are groundwater nitrate concentrations reaching a turning point in some chalk aquifers? Sci. Tot. Env., 408(20): 4722-32, 2010.

Stephens, C., and Quinton, J.: Diffuse pollution swapping in arable agricultural systems. Critical Reviews in Environmental Science and Technology, 39(6): 478-520, 2009.

Storr, E., Adams, R. and Western, A.: How can data from headwater catchments be used to improve runoff and nutrient predictions at larger scales? In Chan, F., Marinova, D. and Anderssen, R.S.(eds) MODSIM2011, 19th International Congress on Modelling and Simulation. Modelling and Simulation Society of Australia and New Zealand:1652-1658, 2011.

Uhlenbrook, S., Roser, S., and Tilch, N.: Hydrological process representation at the meso-scale: the potential of a distributed, conceptual catchment model. Journal of Hydrology 291.3: 278-296, 2004.

Van der Velde, Y., de Rooij, G. H., Rozemeijer, J. C., van Geer, F. C., and Broers, H. P.: The nitrate response of a lowland catchment: on the relation between stream concentration and travel time distribution dynamics, Water Resour. Res., 46, W11534, 2010. doi:10.1029/2010WR009105

Wade, A.J., Whitehead, P.G. and Butterfield, D.: The Integrated Catchments model of Phosphorus dynamics (INCA-P), a new approach for multiple source assessment in heterogeneous river systems: model structure and equations. Hydrol Earth Syst Sci, 6(3): 583-606, doi:10.5194/hess-6-583-2002, 2002

Wade, A.J., Butterfield, D., and Whitehead, P.G.: Towards an improved understanding of the nitrate dynamics in lowland, permeable river-systems: applications of INCA-N, J. Hydrol., 330,185-203, doi:10.1016/j.jhydrol.2006.04.023, 2006

Wade, A. J., Palmer-Felgate, E. J., Halliday, S. J., Skeffington, R. A., Loewenthal, M., Jarvie, H. P., Bowes, M. J., Greenway, G. M., Haswell, S. J., Bell, I. M., Joly, E., Fallatah, A., Neal, C., Williams, R. J., Gozzard, E., and Newman, J. R.: Hydrochemical processes in lowland rivers: insights from in situ, high-resolution monitoring. Hydrol. Earth Syst. Sci.16(11): 4323-42, 2012. doi:10.5194/hess-16-4323-2012

Whitehead, P. G., Crossman, J., Balana, B.B., Futter, M. N., Comber, S., Jin, L., Skuras, D., Wade, A.J., Bowes, M. J., and Read, D. S.: A cost-effectiveness analysis of water security and water quality: impacts of climate and land-use change on the River Thames system. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 371, no. 2002: 20120413, doi:10.1098/rsta.2012.0413, 2013.

Williams, J.R.: The EPIC model. In Computer Models of Watershed Hydrology, Singh VP (ed.). Water Resources Publications: Highlands Ranch, CO (USA); 909–1000. 1995.

Withers, P.J.A. and Lord, E.L.: Agricultural nutrient inputs to rivers and groundwaters in the UK: Policy environmental management and research needs. Soil Use Manage. 14, 186-192. 2002.

7 Tables

Table 1. Attributes of Frome Water Quality monitoring datasets

Dataset	Time Period	Sampling Frequency	Average Number of Observations /Year	Measurements
Long Term Dataset (LTD) CEH/Freshwater Biological Association (Bowes et al., 2011)	1965-2009	Weekly	48	TP,TDP, Nitrate, SRP
High frequency data set (HFD) Bowes et al. (2009a)	1/2/2005 to 31/1/2006	Sub-daily	>1000 (see Table 2 for actual total)	TP,TON, SRP, TSS, instantaneous flows

Table 2. Long term nutrient concentration statistics in the LTD and HFD datasets

Dataset/Nutrient (time period)	Number of Observations	10th Percentile Concentration (mgL^{-1})	Mean Concentration (mgL^{-1})	90th Percentile Concentration (mgL^{-1})
LTD Nitrate (7/1/97-21/11/06)	384	4.6	5.6	6.9
LTD TP (7/1/97-28/2/02)	176	0.13	0.21	0.30
LTD SRP (7/1/97-28/2/02)	183	0.08	0.14	0.20
HFD TON (12/12/04-31/1/06)	1454	4.5	5.5	6.7
HFD TP	2290	0.09	0.17	0.24

(14/1/04-31/1/06)				
HFD SRP (1/2/05-31/1/06)	1340	0.06	0.09	0.14

Table 3. Hydrological model parameters: bounds; and performance metrics (baseline simulation)

	S_{DMAX} (md^{-1})	S_{RZMAX} (m)	K_{SURF} (-)	K_{SPLIT} (-)	K_{GW} (d^{-1})	K_{SS} (d^{-1})
"Expert" value	0.02	0.019	0.08[a]	0.56	0.0011	0.041
Lower Bound	1	1	0	0	0.0001	0.02
Upper Bound	100	500	5	1	0.02	1
NSE (-)	0.80					
MBE (%)	1.00					

[a] K_{SURF} was reduced to 0.012 in the MI scenario

Table 4. Nutrient modelling parameters; from baseline and MI scenarios (only values that were modified from baseline in the MI scenario are shown in parentheses)

Parameter	Nitrate ($mg\ L^{-1}$ N)	SRP ($mg\ L^{-1}$ P)	PP ($mg\ L^{-1}$ P)
C_{OFMIN}	0.4	0.01	0.01
C_{SS}	8.0 (4.0)	0.03 (0.15)	
C_{GW}	4.5	0.22 (0.08)	
$K_{SR}(N)$[a]	0	70	700

[a] units $(mg\ day\ m^{-4})x10^3$

Table 5. Nutrient modelling results; from "Expert" calibration in the baseline scenario (1997-06[a])

Dataset	C_{mod} Mean ($mg\ L^{-1}$)	Error (%)	C_{mod} 90[th] ($mg\ L^{-1}$)	Error (%)	R^2 (-)
LTD Nitrate	6.0	5.4	7.1	3.3	0.04
LTD TP[a]	0.14	-58	0.21	-50	0.02
LTD SRP[a]	0.13	-4.9	0.21	5.0	0.22

[a] Calculated up until 28/2/2002 only

Table 6. Sensitivity Analysis Results (1997-06)

mean (min-max) C and Q	"Expert" (baseline)	5th percentile Behavioural	Median Behavioural	95th percentile Behavioural
Q ($mm\ d^{-1}$)	1.4 (0.46-6.4)	1.1 (0.08-4.5)	1.4 (0.20-5.6)	1.7 (0.41-8.8)
TP C[a] (mgL^{-1} P)	0.14 (0.06-1.9)	0.14 (0.07-0.22)	0.21 (0.11-1.2)	0.23 (0.19-3.9)
SRP C[a] (mgL^{-1} P)	0.13 (0.06-0.22)	0.14 (0.07-0.22)	0.20 (0.10-0.22)	0.22 (0.17-0.38)
Nitrate C (mgL^{-1} N)	6.0 (1.7-7.5)	4.5 (0.73-5.0)	4.8 (2.2-6.6)	5.9 (4.5-7.3)
TP Yield[a] ($kg\ P\ ha^{-1}yr^{-1}$)	0.69	0.72	1.11	1.31

SRP Yield [a] (kg P $ha^{-1}yr^{-1}$)	0.62	0.72	1.10	1.28
Nitrate Yield (kg N $ha^{-1}yr^{-1}$)	33.2	22.8	26.1	32.1

[a] Calculated up until 28/2/2002 only

8 Figure Captions

Figure 1 Schematic map of Frome Catchment showing monitoring points (from Bowes et al., 2009a)

Figure 2 Timeseries plots from the sub-daily HFD dataset from the Frome at East Stoke monitoring point: (2a top pane) Flow data from the catchment outlet comparing the daily mean (DMF) with sub-daily flows by showing the residual; (2b middle) TON and (LTD) nitrate data; (2c bottom) with the results of a two-store MIR model of nitrate also shown (green line), TP, SRP and (LTD) SRP data. The numbered labels (1-5) refer to a classification of different event types described in the text

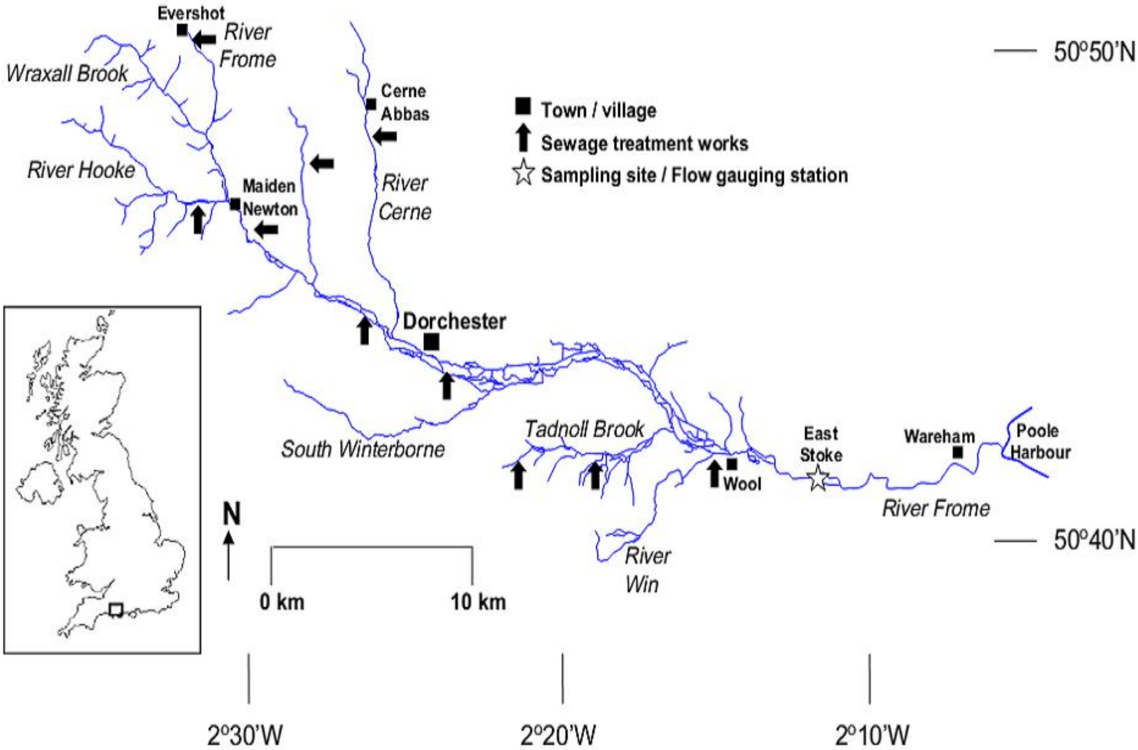
Figure 3 Pie chart showing proportion of 2005-6 Observed TP load from different event and diffuse sources calculated from the HFD dataset

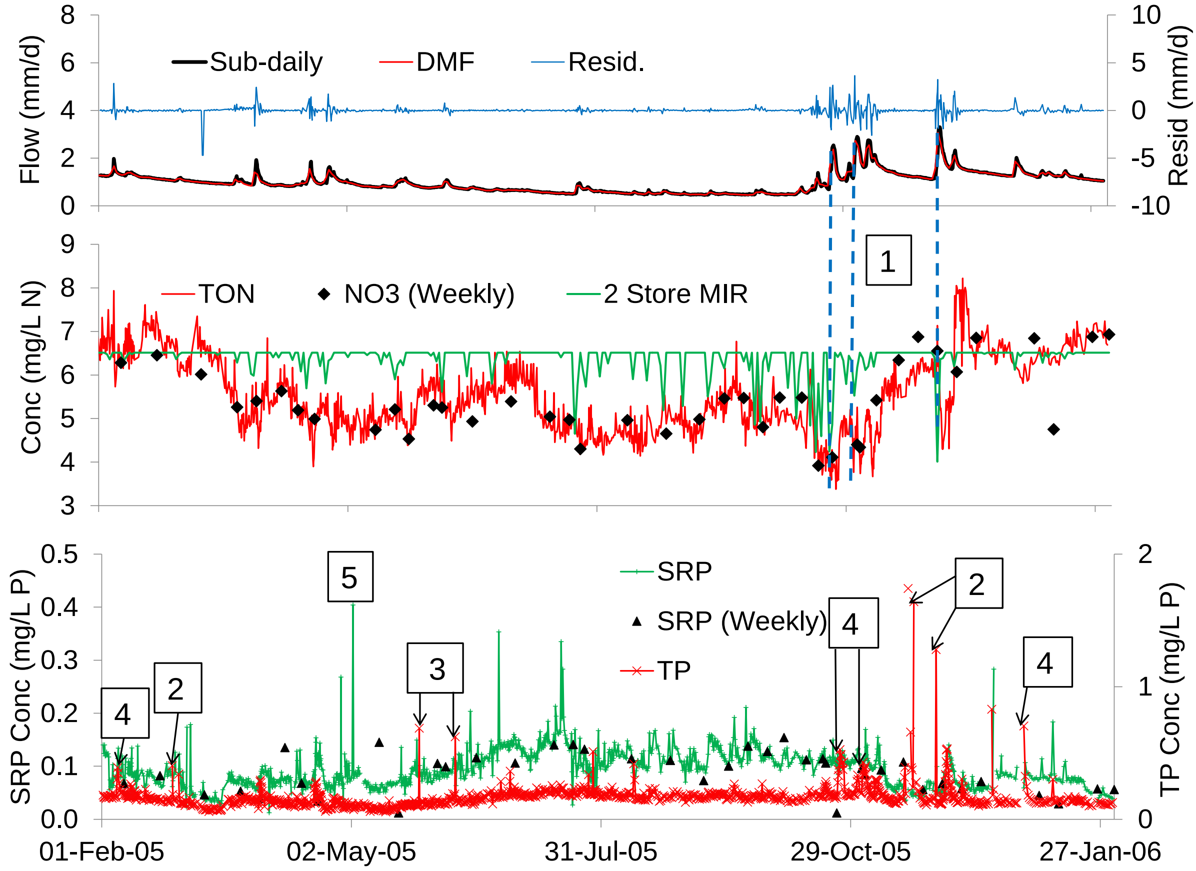
Figure 4 Conceptual diagram of the CRAFT model (top) and a hillslope (bottom), showing the dominant flow and nutrient transport pathways

Figure 5 Timeseries plots of modelled (from “Expert” calibration) and observed (LTD) flows and nutrient data, with the absolute error (AE) (observed-modelled) shown above: (*from top to bottom):* 5a) Flows; 5b) Nitrate; 5c) TP; 5d) SRP. Two years of data shown only.

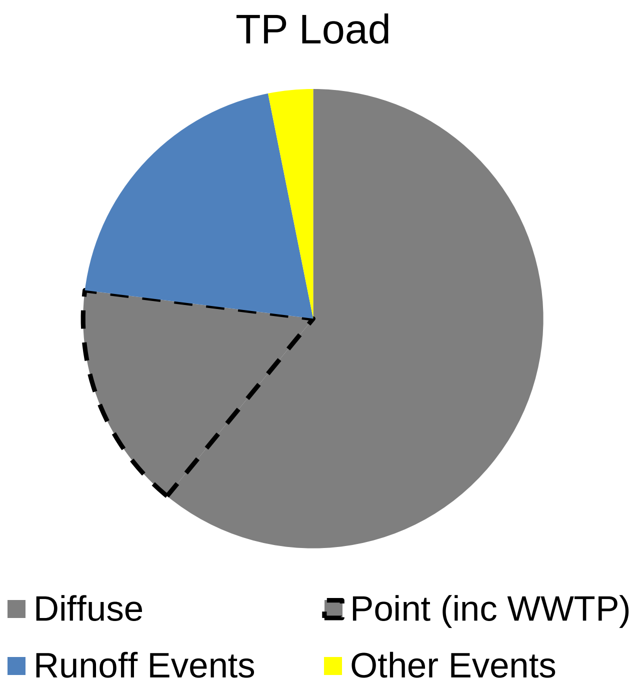
Figure 6 Timeseries plot of modelled (using Monte Carlo sampling to determine parameter values) 5th and 95th percentile and median flows, and the observed flows

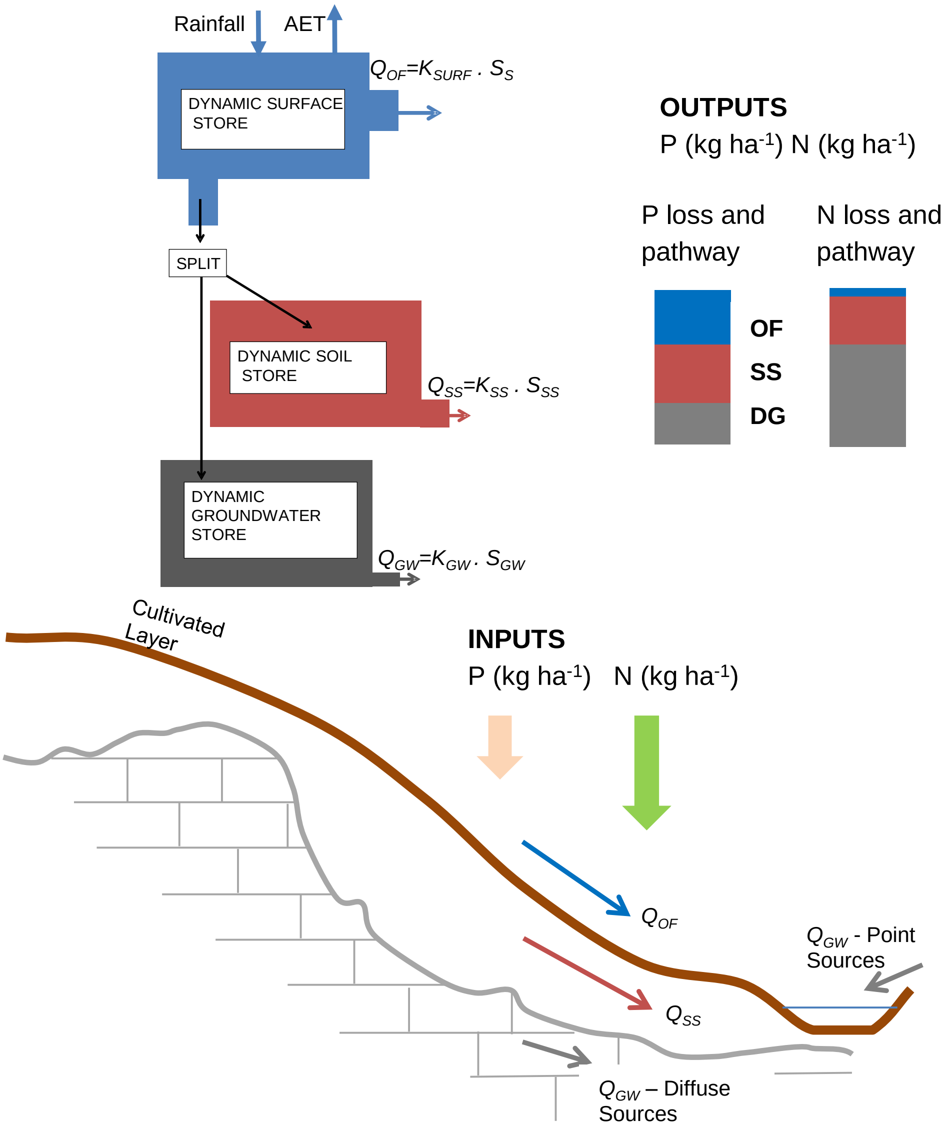
Figure 7 Comparison of the nutrient yields (N and P) from the baseline (left) and MI Scenario (right)


Evershot
River Frome
Wraxall Brook
Cerne Abbas
Town / village
Sewage treatment works
Sampling site / Flow gauging station
River Hooke
Maiden Newton
River Cerne
Dorchester
South Winterborne
Tadnoll Brook
East Stoke
Wareham
Poole Harbour
Wool
River Frome
River Win
N
0 km
10 km
50°50'N
50°40'N
2°30'W
2°20'W
2°10'W

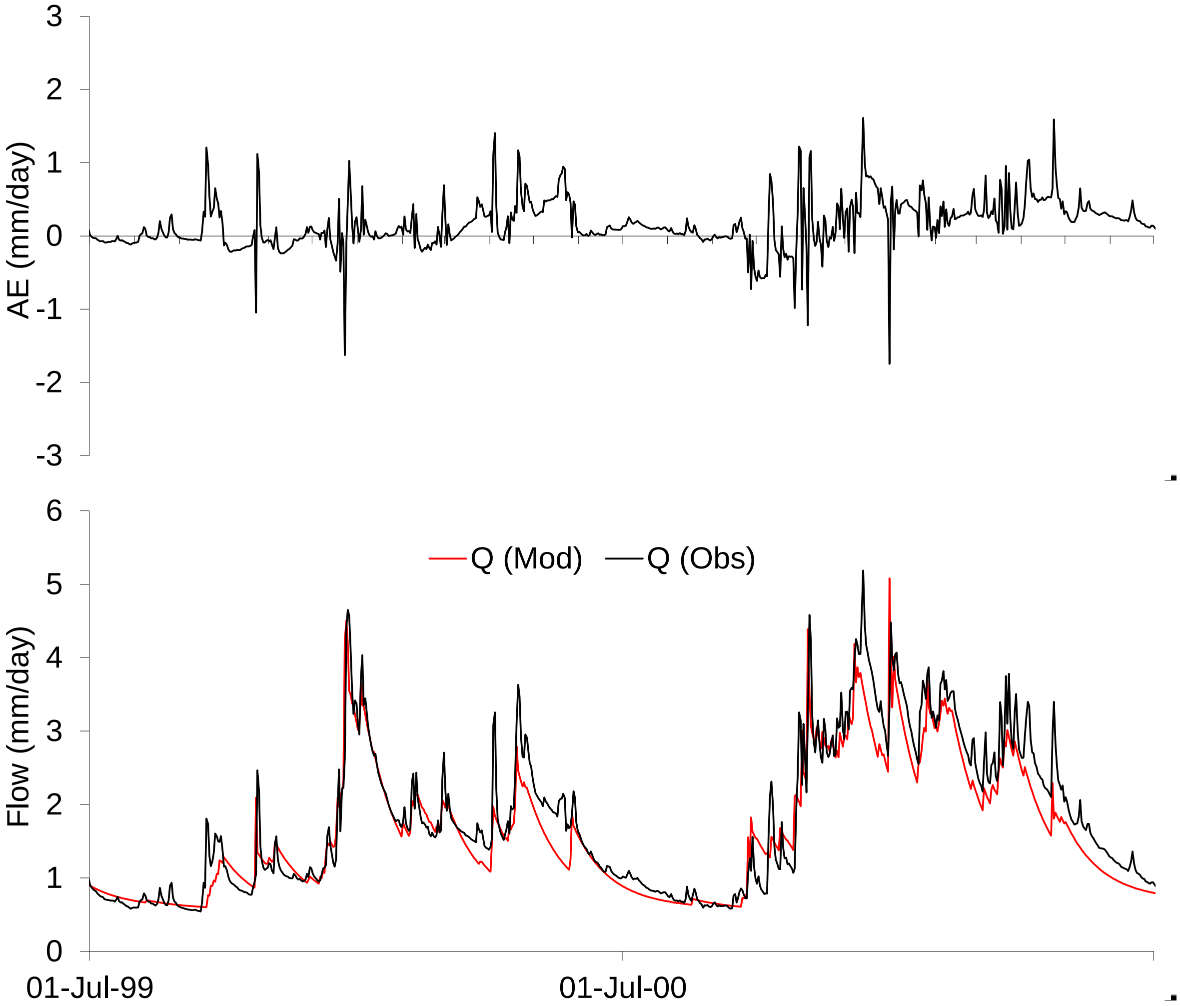

Flow (mm/d)
Resid (mm/d)
Sub-daily
DMF
Resid.
Conc (mg/L N)
TON
NO3 (Weekly)
2 Store MIR
1
SRP Conc (mg/L P)
TP Conc (mg/L P)
SRP
SRP (Weekly)
TP
5
3
4
2
01-Feb-05
02-May-05
31-Jul-05
29-Oct-05
27-Jan-06

830

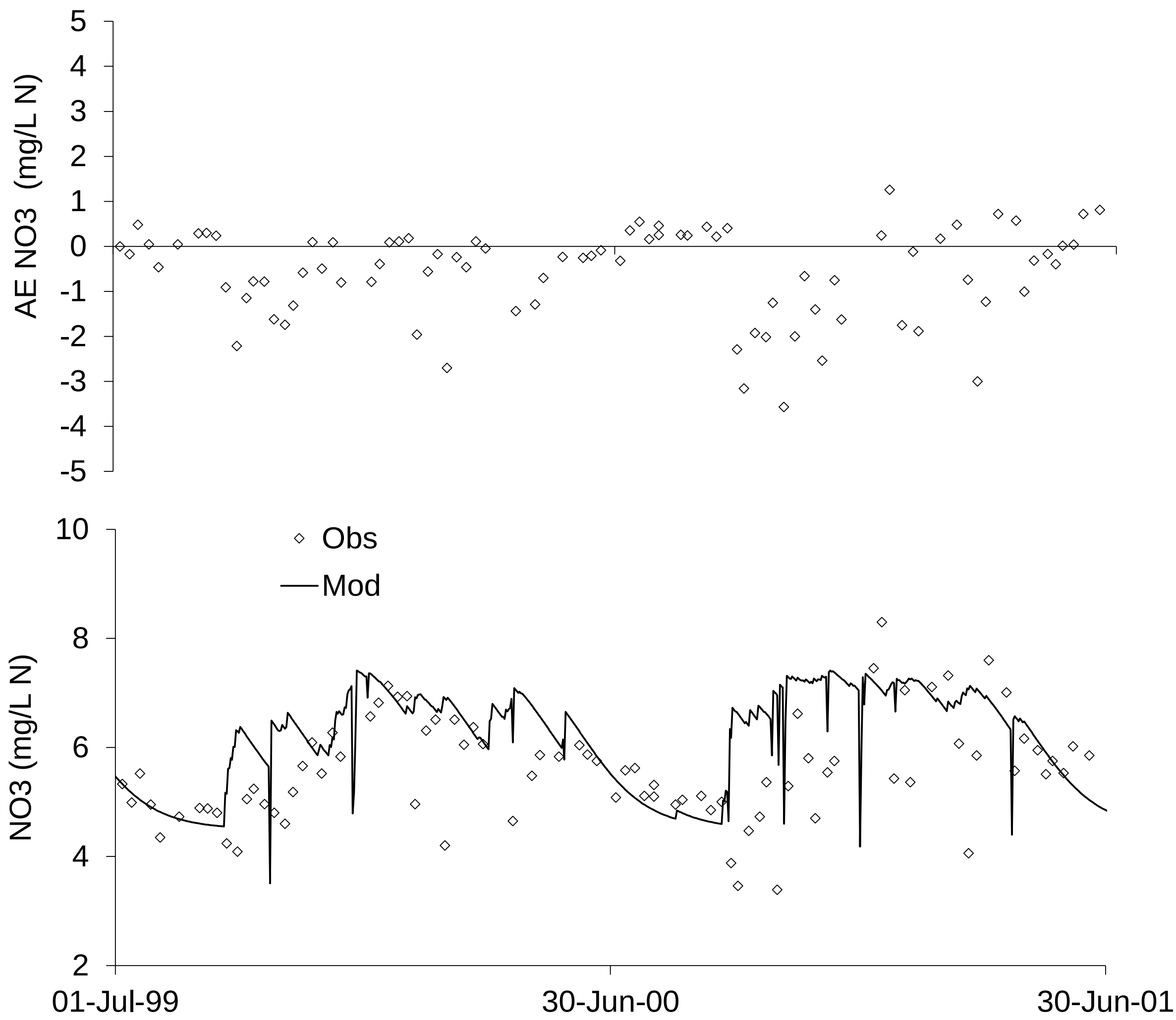

TP Load
Diffuse
Point (inc WWTP)
Runoff Events
Other Events

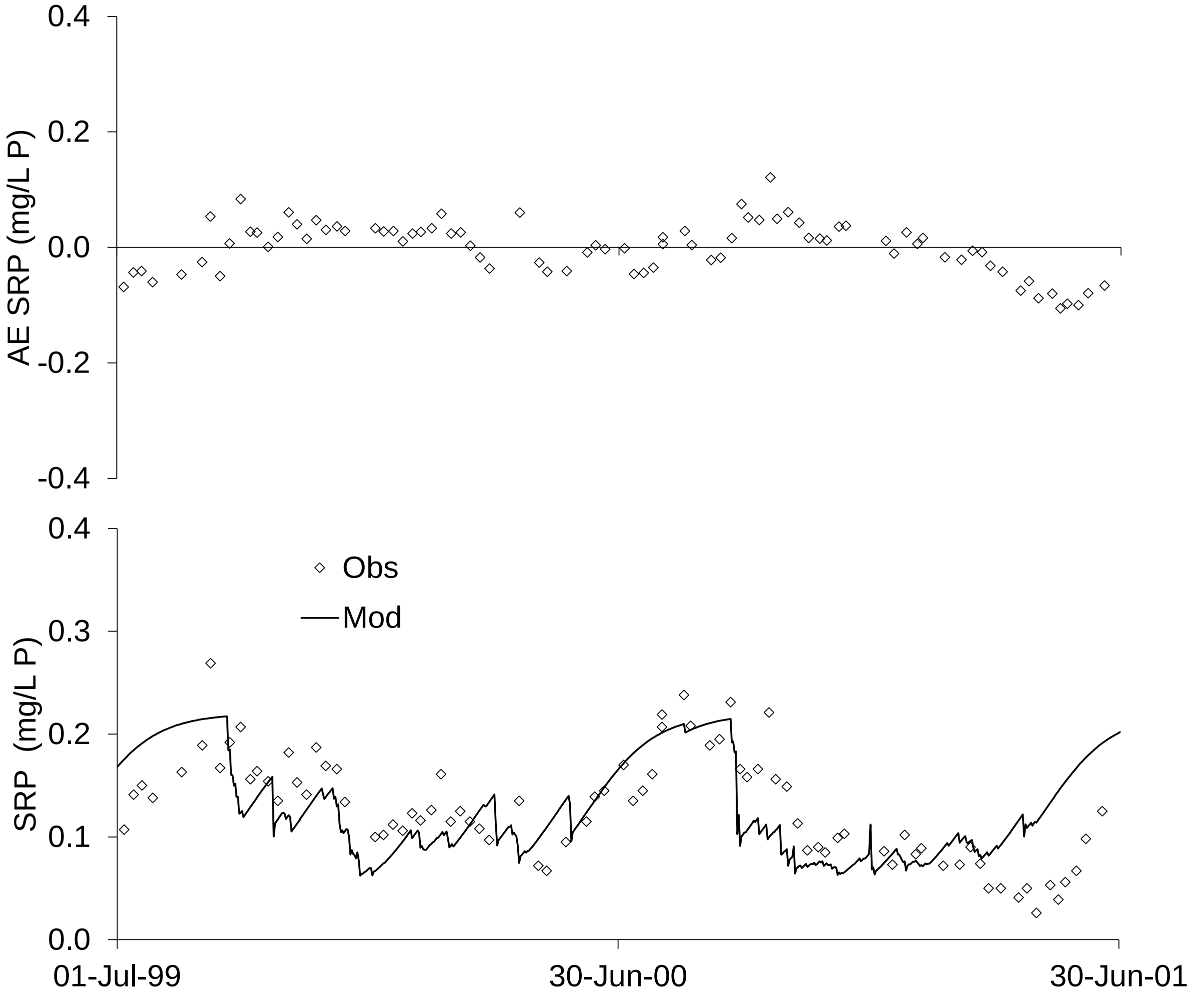

Rainfall
AET
DYNAMIC SURFACE STORE
$Q_{OF}=K_{SURF} \cdot S_S$
SPLIT
DYNAMIC SOIL STORE
$Q_{SS}=K_{SS} \cdot S_{SS}$
DYNAMIC GROUNDWATER STORE
$Q_{GW}=K_{GW} \cdot S_{GW}$
OUTPUTS
P (kg ha-1) N (kg ha-1)
P loss and pathway
N loss and pathway
OF
SS
DG
Cultivated Layer
INPUTS
P (kg ha-1) N (kg ha-1)
Q_{OF}
Q_{GW} - Point Sources
Q_{SS}
Q_{GW} – Diffuse Sources

835

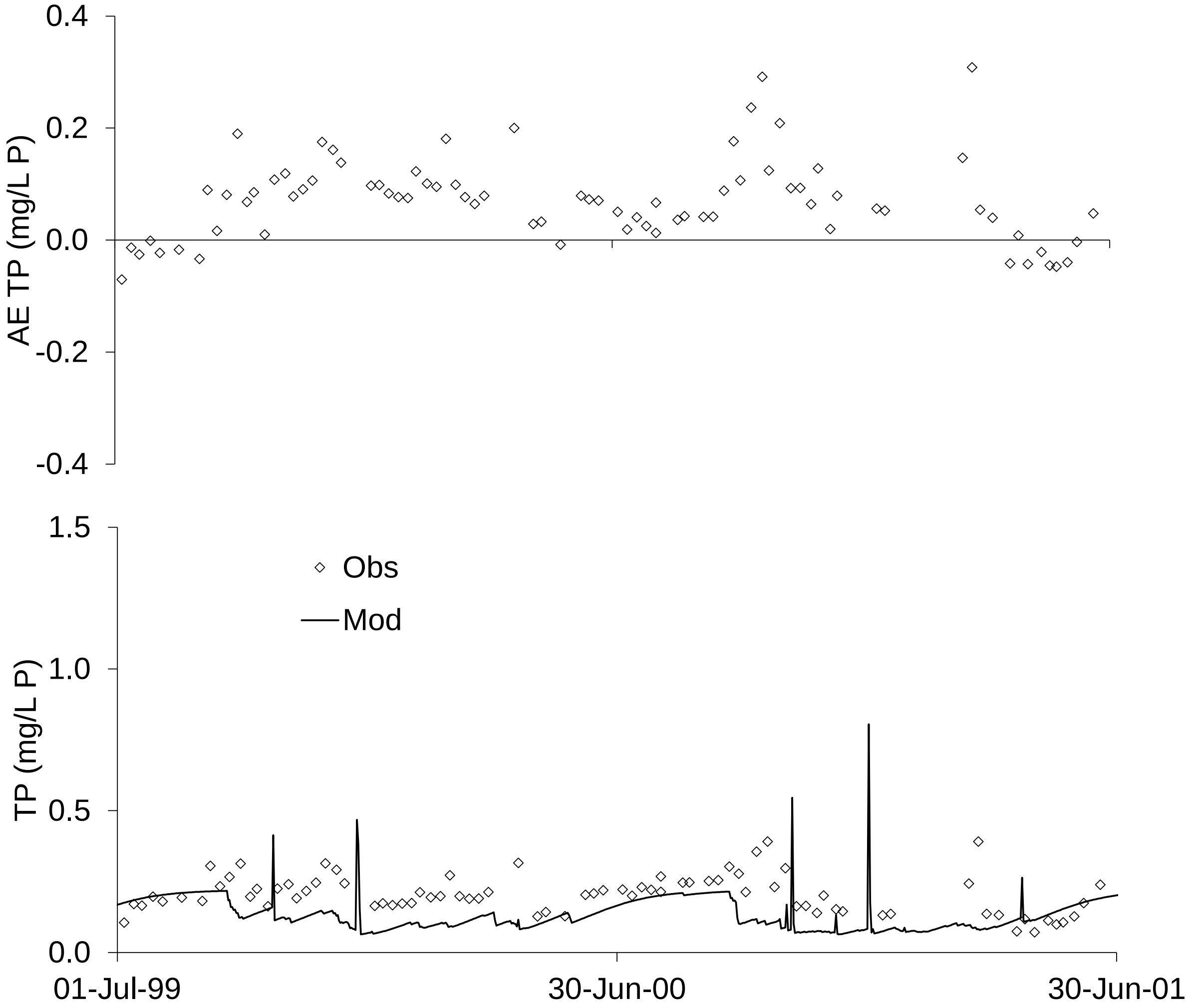


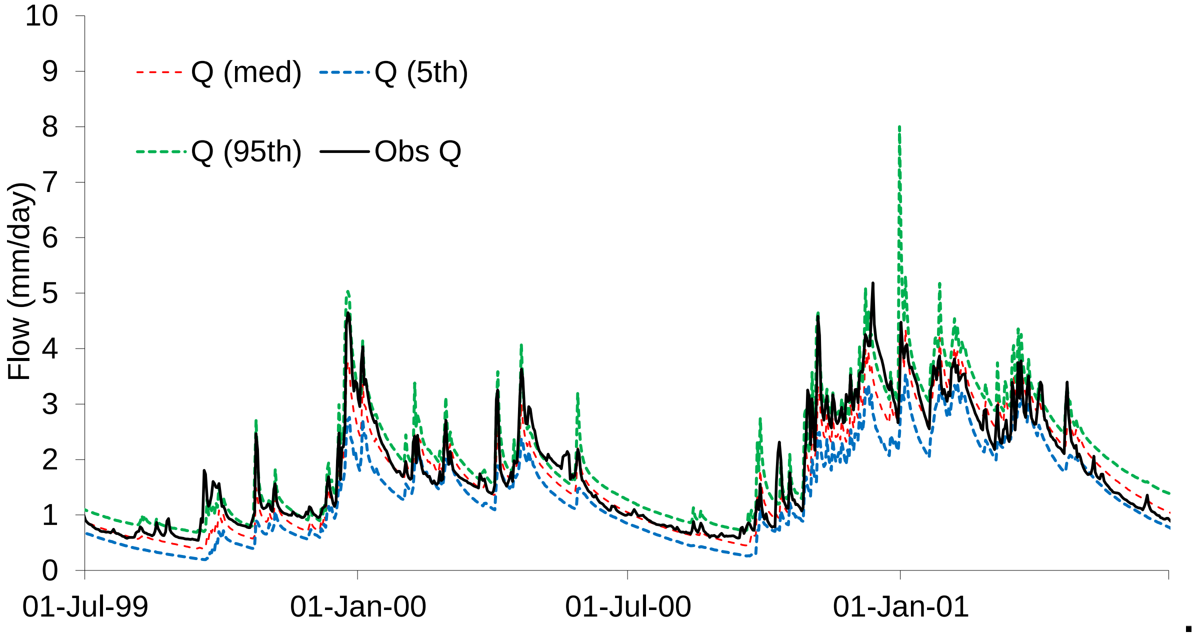
3
2
1
0
-1
-2
-3
AE (mm/day)
6
5
4
3
2
1
0
Flow (mm/day)
Q (Mod)
Q (Obs)
01-Jul-99
01-Jul-00

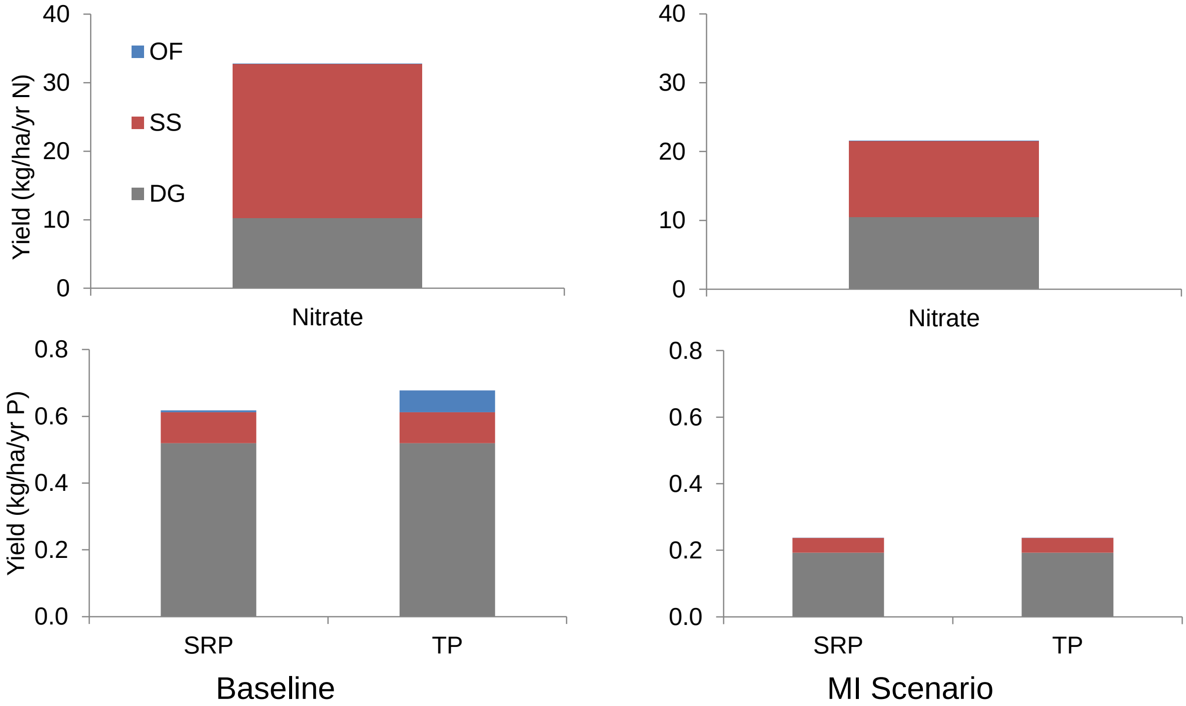

5
4
3
2
1
0
-1
-2
-3
-4
-5
AE NO3 (mg/L N)
10
8
6
4
2
Obs
Mod
NO3 (mg/L N)
01-Jul-99
30-Jun-00
30-Jun-01


0.4
0.2
0.0
-0.2
-0.4
AE SRP (mg/L P)
0.4
0.3
0.2
0.1
0.0
SRP (mg/L P)
Obs
Mod
01-Jul-99
30-Jun-00
30-Jun-01

840


0.4
0.2
0.0
-0.2
-0.4
AE TP (mg/L P)
1.5
1.0
0.5
0.0
TP (mg/L P)
Obs
Mod
01-Jul-99
30-Jun-00
30-Jun-01


Q (med)
Q (5th)
Q (95th)
Obs Q
Flow (mm/day)
0
1
2
3
4
5
6
7
8
9
10
01-Jul-99
01-Jan-00
01-Jul-00
01-Jan-01


40
30
20
10
0
Yield (kg/ha/yr N)
OF
SS
DG
Nitrate
0.8
0.6
0.4
0.2
0.0
Yield (kg/ha/yr P)
SRP
TP
Baseline
40
30
20
10
0
Nitrate
0.8
0.6
0.4
0.2
0.0
SRP
TP
MI Scenario

845