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Using multi-model averaging to improve the reliability of catchment scale nitrogen predictions

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Abstract

Hydro-biogeochemical models are used to foresee the impact of mitigation measures on water quality. Usually, scenario-based studies rely on single model applications. This is done in spite of the widely acknowledged advantage of ensemble approaches to cope with structural model uncertainty issues. As an attempt to demonstrate the reliability of such multi-model efforts in the hydro-biogeochemical context, this methodological contribution proposes an adaptation of the Reliability Ensemble Averaging (REA) philosophy to nitrogen losses predictions. A total of 4 models are used to predict the total nitrogen (TN) losses from the well-monitored Ellen Brook catchment in Western Australia. Simulations include re-predictions of current conditions and a set of straightforward management changes targeting fertilization scenarios. Results show that, in spite of good calibration metrics, one of the models provides a very different response to management changes. This behaviour leads the simple average of the ensemble members to also predict reductions in TN export that are not in agreement with the other models. However, considering the convergence of model predictions in the more sophisticated REA approach assigns more weight to previously less well calibrated models that are more in agreement with each other. This method also avoids having to disqualify any of the ensemble members, which is always sensible.

1 Introduction

Nowadays, mathematical models are often used to assess the impact of changes in boundary conditions on a natural system. More precisely, in the hydro-biogeochemical context, they are used to study the effect of changes in management practices (e.g. fertilization rate), climate or and land-use cover (e.g. clear-cutting, reforestation) on the water and nutrient balances (e.g. Arheimer et al., 2005; Breuer and Huisman, 2009; Zammit et al., 2005). Most of the time, the adopted methodology is to use a single model calibrated to match well with current conditions. Then, some modifications mimicking

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real world changes are done to the relevant boundary conditions resulting in a set of scenarios. The actual scenario prediction is produced by re-running the model with these updated drivers. Impacts can be estimated as the difference between the original model outcomes and the altered ones in either a relative or an absolute way. Optimally, these predictions should be compared to the actual post-change observations to assess their reliability but, in the case of land-use or climate change, this is seldom done as such data are typically not available. Nevertheless, some major concerns arise from this straightforward methodology in catchment scale hydro-biogeochemical model predictions.

First, natural processes involved in the water and nutrient balances (e.g. infiltration, denitrification) are described with a set of equations: the model structure. It primarily consists in a translation of our understanding of natural mechanisms and regulating factors into mathematics. Because of the differences in the hydro-climatic and nutrient contexts between catchments, processes represented in a model can be adjusted by some conceptual parameters that are usually difficult to measure like the inorganic nitrogen retention rate in HBV-N (Arheimer and Brandt, 1998). The corresponding calibration procedure aims at finding the parameter values for which the agreement between observations and simulations is acceptable, based on some goodness-of-fit criteria (e.g. Legates and McCabe Jr, 1999). Although a lot of effort has been put in developing ever more efficient optimization algorithms for the last two decades (Duan et al., 1992; Vrugt et al., 2003), the ability of these models to adequately simulate the impact of changed boundary conditions is of concern (Huisman et al., 2009), especially since predictions are almost never validated against post-change observations (Whitehead et al., 1999).

Second, it is now widely acknowledged that several parameter sets may perform equally well (Beven, 2006) and that the outcome of a successful calibration procedure may indeed not be the actual best result. Therefore, an option to address the uncertainty in predictions, especially in the case of scenario predictions, is to use ensembles of multi-model predictions gathering the information content of several simulations.

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Single-model ensembles regroup predictions obtained with the same model structure whilst altering parameter values and boundary conditions in a Monte-Carlo procedure like the GLUE methodology for example (Beven and Freer, 2001). Nevertheless, part of the predictive uncertainty is also linked to sometimes huge differences between parameterizations, or model structures, developed to address the same issues. As stated by Breuer et al. (2008) this is especially true in the context of hydro-biogeochemical predictions. In order to cope with structural uncertainties, it has become state-of-the-art to consider more than one model simulation of the same system. These ensembles of predictions have been used in the fields of climate, weather, flood forecasting, rainfall-runoff and sub-surface flow and a first multi-model comparison approach targeting agricultural fluxes of nitrogen was published by Diekkrüger et al. (1995). But to our knowledge, the ensemble methodology has only received little interest in the nutrient fluxes context to date, in spite of the demonstrated improvement in prediction reliability. Furthermore, the few available studies, including previous publications by our working group, have only been based on re-prediction (hindcasting) efforts rather than scenario analyses (Exbrayat et al., 2010, 2011; Kronvang et al., 2009). Therefore, we present here an example of the potential advantage of using multi-model predictions to assess the impact of a simple management change on the nutrient balance of a well-monitored mesoscale catchment in South-West Western Australia.

2 Experimental setup

2.1 The Ellen Brook catchment

The Ellen Brook catchment (570 km^2) is located in coastal SW Western Australia and contributes significantly to the water (6 %) and N loads (10 %) entering the Swan-Canning estuary that drains the city of Perth (Viney and Sivapalan, 2001). Most of the catchment has been cleared for agricultural purposes (Swan River Trust, 2007).

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Hydro-climatic conditions are typical of a Mediterranean influence with a mean annual rainfall ranging from 510 to 830 mm yr^{-1} (1989–2006), derived from inverse distance weighted interpolation from the 4 Australian Bureau of Meteorology rain gauges located in the catchment. Intra-annual precipitation is distributed in cool and wet winters and warm and dry summers corresponding to high flow (May–June to September–October) and low to no flow periods (October–November to April–May), respectively (Fig. 1). Because of the sandy nature of the soils, evaporation is high (~ 2 000 mm yr^{-1}) and runoff is mostly generated as a quick and peaky response to rainfall events which explains a five-fold difference between minimum and maximum annual discharge over the study period.

As shown in Fig. 1, about 10 % of the TN flowing out of the Ellen Brook catchment is in the form of dissolved inorganic N (NO_3–N and NH_4–N) derived from animal wastes and fertilizers used for agriculture and private gardens (Swan River Trust, 2007). Dominant organic N forms are either present in dissolved forms of degrading matter or particles composed of plant and animal debris. Concentrations of all N forms rise up during autumn and winter (May–September) because they are flushed with surface runoff. They fall in early spring (September–November) as rainfall, hence runoff, decreases in intensity (Fig. 1). Slight increases in concentrations in December (Fig. 1) may be attributed to either evapotranspiration induced concentration phenomena or animals entering the stream more frequently during these hot periods (Swan River Trust, 2007).

Eutrophication-driven algal blooms have become frequent in the Swan-Canning estuary as a result of nutrient losses from upstream catchments cleared for agricultural purposes such as the Ellen Brook (Swan River Trust, 2009). This has led local authorities to set a target of nutrient loss reduction from upstream catchments of 50 % via different management options: stream bank fencing to reduce animal wastes and erosion, re-vegetation to stabilize river banks, increase community awareness to encourage reductions in fertilizer use, nutrient traps, improved monitoring of hot spots. Meanwhile, a large monitoring effort has been undertaken and more than 900 daily

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samples of total nitrogen (TN) concentrations are available at the Ellen Brook outlet out of a total of 3870 days with runoff between 1989 and 2006. Over this period, mean TN concentration was 2.1 mg N l^{-1} with values ranging from 0.3 to 7.4 mg N l^{-1} with no significant trend in their evolution. This rich dataset allows a reliable application of our model ensemble.

2.2 Model cohort

The more independent the predictions within an ensemble are the more errors tend to cancel each other (Abramowitz and Gupta, 2008). Therefore, in a scenario analysis context multi-model ensembles (MMEs) are preferred to multiple realizations of the same model structure in order to avoid results biased by an eventually inadequate model structure. Accordingly, we setup four conceptual model structures to describe the water and nitrogen balances of the Ellen Brook catchment at a daily time step. The ensemble included LASCAM (Sivapalan et al., 1996a,b; Viney et al., 2000), CHIMP (Exbrayat et al., 2010), SWAT (Arnold et al., 1998) and HBV-N-D (Lindgren et al., 2007). Table 1 summarizes the main features of each model and a short description follows.

The simplest model, LASCAM, only splits the basin into lumped subcatchments over which the land-use cover is considered homogeneous. At each time step, the water balance is solved for each subcatchment and surface runoff, sub-surface flow and baseflow discharge into the corresponding stream. Since it has been developed for semi-arid and hot regions where temperature is not a limiting factor, LASCAM does not require temperature input. Therefore, only substrate availability governs the represented soil N turnover processes that affect the three considered N-species (NO_3–N, NH_4–N, and TN): residue decay, plant harvest, mineralization, volatilization, plant uptake, nitrification, denitrification and fixation (Viney et al., 2000). Nutrients discharging from land into the stream are routed to the catchment outlet.

CHIMP is a more complex semi-distributed model which further divides the subcatchments into land-use classes (Exbrayat et al., 2010). Water and nutrient balances are calculated for each of them before their outcome is weighted by the respective

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relative area over the sub-catchment. The same N-species than in LASCAM are considered after recent implementation of an organic N store (Exbrayat et al., 2011) but temperature has a positive effect on the soil N turnover processes of plant uptake, nitrification, denitrification, fixation, mineralization and immobilization. In-stream denitrification and nitrification processes can also occur.

The well-known SWAT model adopts a more detailed spatial distribution scheme by considering each single combination of land-use and soil type as an independent Hydrological Response Unit (HRU). Water balance and different moisture- and temperature-controlled N turnover processes are simulated for each HRU: plant uptake, residue decay, mineralization, nitrification, volatilization, denitrification, fixation and leaching. Re-infiltration from stream is also allowed along algal respiration and uptake. Amongst our four models, SWAT requires the most data and the multiple input files were directly generated from GIS data (Olivera et al., 2006).

Whereas the three previously described models are semi-distributed with nested subcatchments discharging into another only via stream flow, the fully distributed HBV-N-D (Lindgren et al., 2007) simulates the water and nutrient balances for each 100×100 m grid cell across the Ellen Brook catchment. Each pixel has its own land-use class with corresponding parameters and each grid cell flows into the adjacent downstream one following a single-flow direction algorithm. HBV-N-D only considers TN and a single retention process assumed to represent the net effect of denitrification, uptake and sedimentation as a function of temperature and substrate availability.

Because of this difference in the spatial representation of the catchment within HBV-N-D, there is a massive difference of up to 3 orders of magnitude in the number of considered smallest spatial units over the Ellen Brook catchment (Table 1). Required boundary conditions and spatial disaggregation scheme within each model are summarized in Table 1, along with our catchment-specific setup properties. Discrepancies in considered nutrient species, and relevant turnover processes, represent a sample of the large structural differences that exist in hydro-biogeochemical models (Breuer et al., 2008).

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The setup process of the different models to simulate the behaviour of the Ellen Brook catchment is similar (but not identical) to the one previously used by Exbrayat et al. (2011) and is only briefly described hereafter. First, the hydrological component of each model was calibrated with the SCE-UA (Duan et al., 1992) by reducing the root-mean-square-error (RMSE) of observed vs. predicted daily runoff between 1989 and 1997. Then, by keeping the calibrated hydrological parameters fixed, parameters governing the different N mobilization and transport processes were also optimized with the SCE-UA algorithm set to minimize the RMSE of daily TN loads years 1998 to 2006 were used for validation and scenario purposes.

One of the ways to fulfil the requirements of the Swan Canning Water Quality Improvement Plan is to reduce diffuse source of total nitrogen (TN) that constitutes fertilizer application (Swan River Trust, 2007). Here, in order to illustrate the reliability ensemble averaging (REA) philosophy with a simple example, we apply some very straightforward scenarios of changing agricultural management practices (i.e. fertilizer reduction) over the catchment for the period 1998 to 2006. For each new simulation, the current fertilizer application rate of 30 $\mathrm{kg\,N\,ha^{-1}\,yr^{-1}}$ in the form of ammonia (Zammit et al., 2005) is stepwise decreased by 10 % of its original value and the models are re-run for the validation period. Then, we apply the REA weighting scheme described hereafter to all single predictions.

2.3 Reliability ensemble averaging

Previous studies on multi-model averaging techniques set in a variety of environmental modelling contexts have demonstrated that the simple mean of a MME usually outperforms its members taken separately in terms of goodness-of-fit metrics (Georgakakos et al., 2004; Shamseldin et al., 1997; Viney et al., 2009). However, it has also been shown that giving more weight to the already better performing members tends to provide an overall more reliable prediction (Exbrayat et al., 2010; Krishnamurti et al., 1999; Viney et al., 2009). In this case, a "performance" coefficient R_B weights each single prediction according to either a goodness-of-fit metric (e.g. RMSE), multiple-linear

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regression methods or more sophisticated techniques like the Bayesian Model Averaging (Raftery et al., 2005).

Following this, Giorgi and Mearns (2002) proposed to also consider the agreement between the models in response to the same changes in boundary conditions in the weighting scheme. The surrounding philosophy is that the influence of a very well calibrated model on the final prediction should be dampened if it provides a completely different response than the other models to the same changes. In that sense, outlying predictions are penalized by the introduction of a "convergence" coefficient R_D favouring more central predictions in the weighting scheme. Although primarily designed for climate studies, the so called Reliability Ensemble Averaging (REA) method has been recently adapted to scenario analyses of land cover change impact on runoff (Huisman et al., 2009). Put in a mathematical way, the final weight R_i assigned to each member of the MME can be summarized as

$$R_i = R_{B,i} \cdot R_{D,i} = \left(\frac{\varepsilon}{|B_i|}\right) \cdot \left(\frac{\varepsilon}{|D_i|}\right) \quad (1)$$

where B_i and D_i are measures of the performance and convergence for model i, respectively. The term ε corresponds to a measure of the variability in TN export, expressed as the difference between the highest and smallest observed values. Following Huisman et al. (2009), B_i corresponds to the model bias in simulating present-day TN export, i.e. the relative difference between simulated and observed TN export on days with measurements. The term D_i is a measure of the distance between the change predicted by a model i, and the REA average change such as

$$D_i = \Delta\mathrm{TN}_i - \frac{\sum_{i=1}^{N} R_i \cdot \Delta\mathrm{TN}_i}{\sum_{i=1}^{N} R_i} \quad (2)$$

where $\Delta\mathrm{TN}_i$ is the relative change of TN export predicted by model i, and N the number of models in the ensemble. The REA average change is not known beforehand and

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it is obtained iteratively following Giorgi and Mearns (2002). One of the key points of the REA method is that $R_{B,i}$ or $R_{D,i}$ are set to 1 whenever B_i or D_i are smaller than ε, respectively. Assuming that the probability density function of the change is somewhere between uniform and Gaussian, a 60–70 % confidence interval is represented by the REA average change plus and minus the weighted root mean square difference (RMSD) such as

$$\mathrm{RMSD} = \left(\frac{\sum_{i=1}^{N} R_i \cdot \left(\Delta TN_i - \overline{\Delta TN} \right)^2}{\sum_{i=1}^{N} R_i} \right)^{1/2} \quad (3)$$

3 Results

Calibration and validation metrics are presented in Table 2. According to the RMSE, the LASCAM model performs the best for both periods whilst CHIMP gives the closest average daily TN export predictions as compared to the observation data. CHIMP and HBV-N-D prediction quality increase between calibration and validation whilst the opposite is observed for LASCAM and SWAT.

Generally, models simulated less TN export during validation than during calibration. The highest TN export is simulated by SWAT with ∼131 and ∼118 $\mathrm{t\,N\,yr^{-1}}$ during calibration and validation, respectively. This corresponds to almost 4 times more export than HBV-N-D predictions (∼34 and ∼31 $\mathrm{t\,N\,yr^{-1}}$). According to Fig. 2 which represents the exceedance probability of daily TN losses simulated by the models, it seems that this difference is due to some rare events of intensive TN export predicted by SWAT. Meanwhile, LASCAM and CHIMP are in a better agreement with each other over the whole period. This is especially true for the simulated export rates of ∼83 and ∼85 $\mathrm{t\,N\,yr^{-1}}$ for the calibration period by LASCAM and CHIMP, respectively. Corresponding values of ∼60 and ∼69 $\mathrm{t\,N\,yr^{-1}}$ for the validation period differ a bit more

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but are still the most similar amongst all the models. As illustrated in Fig. 2, LASCAM simulated more frequent daily TN exports greater than $1\,\mathrm{t\,N\,d^{-1}}$ than CHIMP whereas CHIMP's higher probability of lower N losses and less frequent no flow occurrence explains its higher average yearly TN export.

Figure 3 summarizes TN export changes for each model. All the members of the ensemble present a sensible diminution of the TN export after reduction in the fertilizer application. The responses of LASCAM, SWAT and HBV-N-D to the changes in management practices are comparable to each other, with a total reduction towards less than 10 % when no fertilizer is applied. Conversely, CHIMP presents a totally different behaviour with a reduction of up to 80 % of its initially simulated TN export. The simple mean provides intermediary predictions towards a ∼25 % TN export reduction with no fertilizer. On the other hand, the REA average change is well in agreement with HBV-N-D, LASCAM and SWAT with a reduction in TN export below 10 %. The shaded area in Fig. 3 represents ∼60–70 % of the uncertainty (REA average ± RMSD) of the change and always includes these 3 models but not CHIMP. The simple averaging scheme is not in the uncertainty bounds of the REA for reductions of more than 30 % in fertilization, and moves further away from it when the reduction increases.

4 Discussion

Consistently with previous work in hydro-biogeochemical modelling by Breuer et al. (2008), Exbrayat et al. (2010) or Kronvang et al. (2009), discrepancies between model structures (Table 1) driven by a homogeneous dataset of boundary conditions are a source of large predictive uncertainty. Interestingly, the more lumped models LASCAM and CHIMP seem to perform better in estimating the nutrient losses than the more distributed ones. This may be due to a conceptualization of the N cycle more adapted to the Ellen Brook conditions. For example, LASCAM has originally been developed to predict the water, salt and nutrient balances in SW Western Australian catchments including the Ellen Brook (Viney et al., 2000; Zammit et al., 2005). Nonetheless, since

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our aim is to quantify a relative change in total TN export in response to reductions in fertilization rates, we do not reject any of the models for our application.

The most striking feature in Fig. 3 is the behaviour of the CHIMP model during the scenario analysis. In spite of its good calibration and validation results, CHIMP simulates a reduction of up to 80 % in TN export while all the other models seem to be more in agreement with a total reduction not higher than 10 % of the current TN export. Therefore, we could attribute the acceptable calibration results of CHIMP as the outcome of a successful curve-fitting exercise (Wade et al., 2008). Further, because of the outlying position of CHIMP, the simple mean provides a final prediction equivalent to an almost 25 % reduction in nitrogen losses when no fertilization occurs. However, the trust we can put in this projection is questionable since it is not really in agreement with any of the single projections and that its intermediary position is merely a result of very different but equally weighted projections.

On the other hand, when the agreement between models is introduced into the REA weighting scheme, the converging responses of the LASCAM, SWAT and HBV-N-D models to changed conditions provide a significantly different final prediction than the former simple averaging scheme. Similarly to some of the well calibrated models in Huisman et al. (2009), the outlying position of CHIMP decreases its reliability in the final weighing scheme. Conversely, and in spite of their relative poorer ability to match current conditions, SWAT and HBV-N-D "attracts" the final averaged prediction by being consistent with each other, and LASCAM, in their relative response to the management scenarios. This results in a final REA average prediction that looks more consistent with most of the single models.

Of course, one could argue that the ensemble approach is not entirely justified in our case because LASCAM is a well calibrated model that also presents the expected behaviour during scenario analyses. However, contrary to the other models, LASCAM was primarily developed and tested to simulate water and nutrient fluxes in this particular catchment (Viney et al., 2000). In another application case, it is not sure that the chosen model structure would have been developed over several years to predict

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the hydro-biogeochemical fluxes of the catchment of interest, nor that there would be enough monitoring data to support model quality assessment. Similarly, although we agree that CHIMP's source code needs a thorough inspection in a near future, detection of probable quirks in its structure would not have been possible without comparing its predictions with other models in scenario analyses.

Nonetheless, the results obtained with the adopted averaging method are a good demonstration of its ability to extract the most reliable content of information from each ensemble member (Giorgi and Mearns, 2002). This is very valuable in the frame of hydro-biogeochemical predictions (Breuer et al., 2008) and could be helpful for application cases in which the absence of monitoring would make it hard to identify the most appropriate structure (Huisman et al., 2009) like land-management scenarios or prediction in Ungauged Basins (Sivapalan, 2003). This is especially true since we usually rely on models developed and calibrated for stationary and not changing conditions (Milly et al., 2008; Sivapalan et al., 2011).

5 Conclusions

Through our straightforward example of fertilization rate reduction we demonstrated the advantage of using a multi-model ensemble to lower the risk of relying on a single, maybe subjectively chosen, model structure. This is a real advantage since the actual effects of different changes (management, climate) are not yet known, making the evaluation of model quality impossible. So far, REA and similar averaging schemes have been primarily been applied in climate and hydrological sciences. We see a great potential of this technique in other fields of environmental modelling where the structural uncertainty of models used for predictions is large and rarely addressed.

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Table 1. Model characteristics.

Model	Smallest spatial unit	Climate forcing	Nutrient forcing	N species	# spatial units
LASCAM	Subcatchment	Daily P and annual PET	Rainfall concentration, fertilizer application	NO_3–N, NH_4–N, Organic-N	29
CHIMP	Land-use class	Daily P, T and PET	Rainfall concentration, fertilizer application	NO_3–N, NH_4–N, Organic-N	108
SWAT	HRU	Daily P, maximum and minimum daily T	Rainfall concentration, fertilizer application	NO_3–N, NO_2–N, NH_4–N, Organic-N	608
HBV-N-D	Grid cell	Daily P and T and PET	Rainfall concentration, leaching coefficients, fertilizer application	TN	~ 57 000

P: precipitation,
PET: potential evapotranspiration,
T: air temperature,
HRU: hydrological response unit

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Table 2. Model calibration (1989–1997) and validation (1998–2006) results.

Model	RMSE ($gNha^{-1}d^{-1}$)		Average TN export on sampled days (tNd^{-1})		Total TN export ($tNyr^{-1}$)	
	Calibration	Validation	Calibration	Validation	Calibration	Validation
Observations	–	–	0.53	0.41	–	–
LASCAM	5.4	7.1	0.51	0.48	83.0	59.7
CHIMP	10.8	9.9	0.52	0.36	84.9	69.0
SWAT	18.4	26.2	0.55	0.65	131.1	117.7
HBV-N-D	14.3	10.4	0.24	0.21	34.3	31.3

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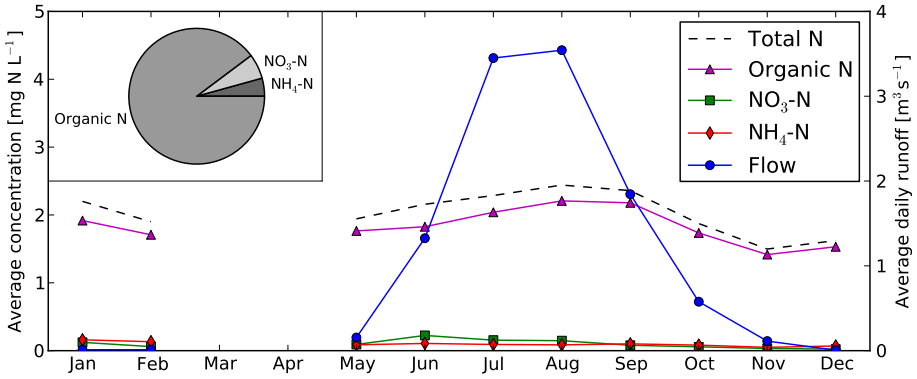

Fig. 1. Seasonal cycle and relative contribution of different species to TN (pie chart) in the Ellen Brook (1989–2006). Missing values in March and April correspond to no flow periods..

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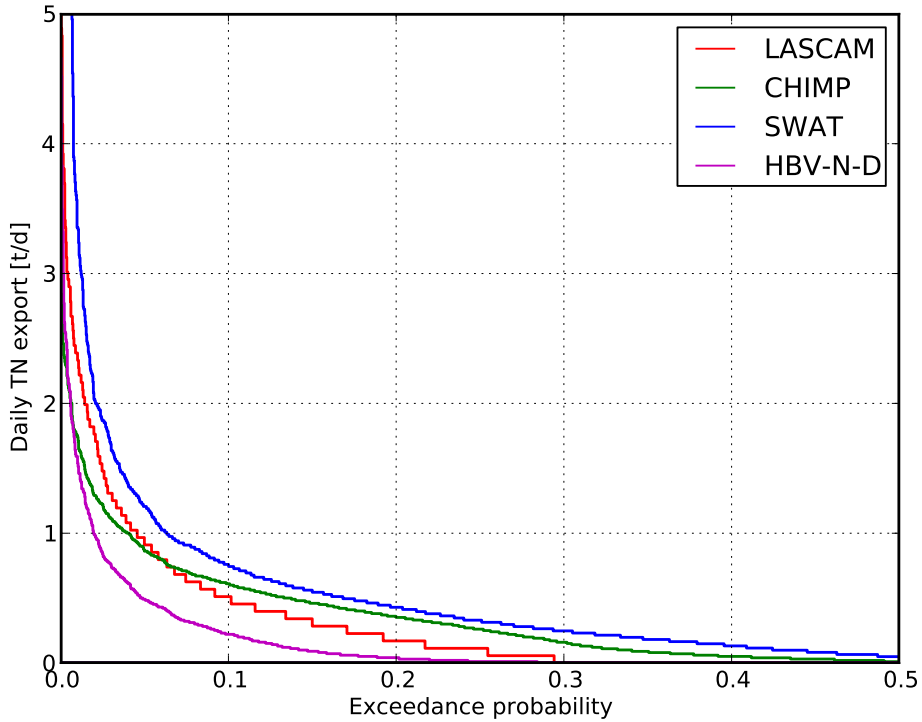

Fig. 2. Exceedance probability of daily TN exports as predicted by the models during the validation period.

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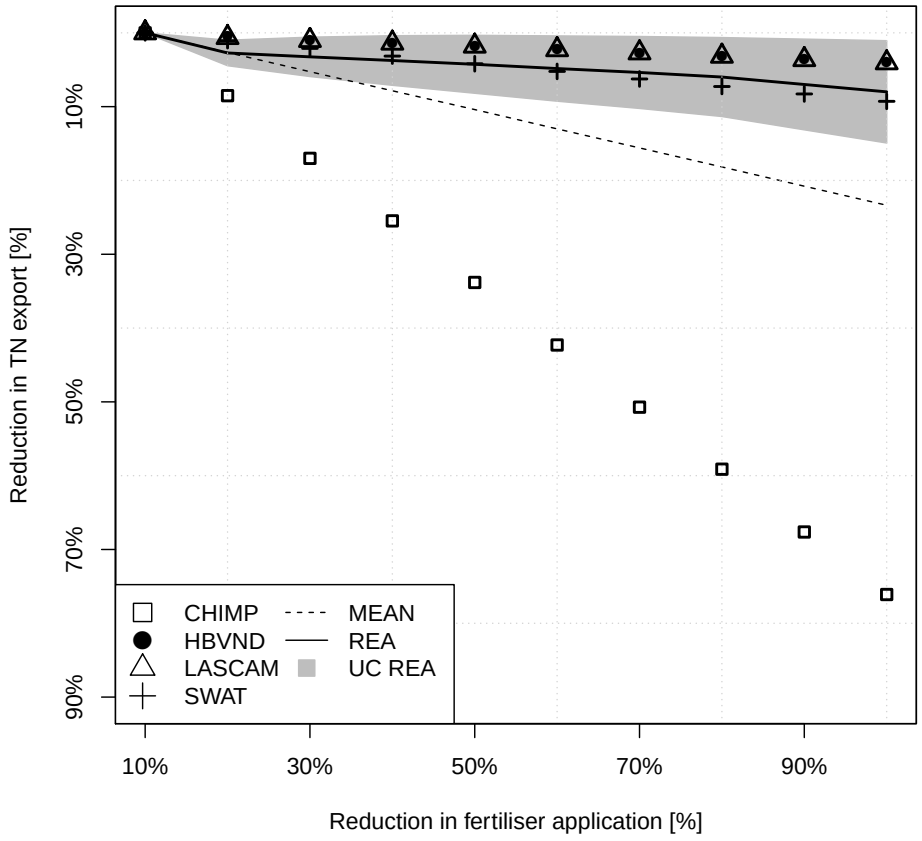

Fig. 3. Evolution of fractional TN export (a proportion of the initial TN export) with different scenarios of fertilization reduction.

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