

Parameter sensitivity analysis of the JAMS/J2000-S model to improve water and nutrient transport process simulation - a case study for the Duck catchment in Tasmania

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The spatially distributed and process-oriented water and nutrient transport model JAMS/J2000-S was used to quantify nitrate transport process dynamics in the meso-scale, humid Duck catchment in Tasmania, Australia. As shown by previous studies, the model was successfully calibrated and validated based on the comparison of model results with observed water volumes and monthly monitored nutrient concentrations.

However, model approaches using large numbers of calibration parameters imply parameter uncertainties which might affect model results significantly. In particular in catchments with relative low nutrient concentrations, parameterisation needs to be done carefully assuming that little changes in parameter settings have significant influence on the simulated outputs. Observations in Tasmanian catchments showed that nitrogen concentrations are considerably low, already catchments with concentrations of less than 1 mg/l NO₃-N are being reported as 'impacted.'

The fully distributed model JAMS/J2000s has been previously applied for the Tasmanian Duck catchment to assist water resources management and to improve the understanding of diffuse source pollution and its contribution from different pathways. One of the key questions of this study was to find out if the model is capable to simulate these low concentrations with a reasonable quality and to quantify.

As a supplement to this first study now a regional parameter sensitivity analysis was applied for the Tasmanian Duck catchment to:

- (i) identify those parameters that significantly influence model results in terms of simulated nitrate concentration at the catchment outlet,
- (ii) test the model's suitability and applicability for the specific Tasmanian conditions, and
- (iii) provide feasible parameter ranges for Tasmanian test catchment conditions allowing the regionalized application of the developed model.

The paper present the results obtained in the Duck catchment, the applied methodology for the sensitivity analysis along with the findings obtained with this procedure. The results of the study showed that JAMS/J2000s was able to accurately simulate the hydrological dynamics in the Duck catchment. The comparison of simulated and observed runoff in the validation period resulted in a Nash-Sutcliffe efficiency of 0.7 and a coefficient of determination of 0.91. The most obvious feature was a slight overprediction of the runoff volume in particular at the beginning of the wet period. The comparison of the simulated N-concentration at the catchment outlet with a number of observations did also show the principle suitability of the model to reproduce the nitrogen turnaround processes in the basin.

The sensitivity analysis of six model parameters, based on a Monte-Carlo-Analysis of 2400 model runs showed that only three parameters considerably affect the simulation of the N-concentration. These were the parameters which are responsible for the mobilization of nitrogen, whereas the three insensitive parameters are responsible for the distribution and mixing of nitrogen in the soil profile. An additional sensitivity analysis output was obtained for one parameter which was responsible for very poor model results when set to values which were exceeding a specific threshold. This behaviour gives an indication for a potential structural model problem for either the Tasmanian conditions or in general which needs to be addressed in further studies. The overall outcome of the study showed that the JAMS/J2000s model seems to be very suitable for the assessment and simulation of water and nutrient transport processes in the Tasmanian Duck catchment. Nevertheless, the study showed that the model still has some systematic shortcomings which need more research and testing in future projects in Tasmania and other regions.

Keywords: *Sensitivity analysis, Monte Carlo simulations, Water quality modelling, Tasmania*

1. INTRODUCTION

The identification of non-point nutrient sources and the importance of their processes in conjunction with management actions are essential for the development of catchment scale management plans. In practise, the detection of these sources remain critical as catchments usually comprise heterogeneous catchment characteristics and various land use management options resulting in multiple pathways, process interactions, and a strong non-linear behaviour of flow and associated nutrient transport. Sound monitoring together with calibrated and validated spatial distributed and process-oriented models offer the potential to study these effects (Jorgensen *et al.*, 2007). Models can assist therefore in a variety of planning steps for water resource management. For water resource management in Tasmania, four main planning steps are usually carried out. First, information on current water quality conditions of impaired freshwater systems and estuaries are required that also includes analysis on cause-effect relationships for their impacts. The next step is setting of resource condition targets (RCTs) to scale water quality objectives and benchmarking targets for improvements including an additional water resources management step. The selection of appropriate tools and mechanism to implement on-ground management actions is complemented by a review cycle that allows measuring the progress.

The fully distributed model JAMS/J2000s has been previously applied for the Tasmanian Duck catchment (Bende-Michl *et al.* 2007). To assist water resources management, it was used to better understand and to quantify diffuse source pollution and its contribution from different pathways. Based on the model results, efficient nitrogen reduction measures should be developed for legislative reasons. Model parameterisation and calibration has been carefully carried out as the nutrient concentrations observed in Tasmanian catchments are relative low compared to European and North-American conditions. The key questions of this study were to find out if the model is capable of simulating these low concentrations with a reasonable quality and to quantify the sensitivity of the single model parameters controlling the nutrient concentration in the runoff.

2. METHOD

2.1. Spatial Distributed Model JAMS

JAMS (Jena Adaptable Modelling System) is a modular object-oriented framework system (Kralisch and Krause 2006) developed at the University Jena, Germany. It includes a variety of tools and modules for hydrologic and solute landscape analysis on various spatio-temporal scales. The JAMS framework was used to build different models like the process oriented hydrological model J2000, the simplified water balance model J2000g, and the distributed, process oriented nutrient transport model J2000s including modules for simulation of land use management (Krause 2001, Krause *et al.* 2006, Bende-Michl *et al.*, 2006, Fink *et al.*, 2007). It also includes modules for model optimisation and sensitivity/uncertainty analysis as well as 2D/3D visualisation tools. JAMS can be used in a problem-oriented fashion as the user can select and define a suitable set of modules to be used for a particular application.

The hydrological and solute modules are designed for process oriented landscape analysis. The hydrological part comprises methods for input data regionalisation, radiation calculation, and calculation of potential evapotranspiration according to Penman-Monteith. The hydrological processes which are considered are interception, snow accumulation and ablation, horizontal differentiated soil-water balance, ground-water balance, runoff generation and explicitly computed lateral surface and subsurface flows and flood routing in the catchment's river network (Krause *et al.* 2006).

The nutrient transport routines were mainly adopted from SWAT (Arnold 1998) and are coupled to the hydrologic components of J2000 (see Figure 1). The nutrient modules include process components for simulating soil temperature, crop growth and nitrogen turnover according to Neitsch *et al.* (2002) and Williams *et al.* (1984) with some minor adaptations. Five different soil N pools are considered in order to allow modelling of different N inputs (e.g., mineral fertiliser, organic manure) and N transformations between these pools. N reduction is modelled by a dynamic crop growth module and subsequent N uptake of plants (residues and yield) as well as through denitrification and volatilisation. The influence of soil temperature and soil moisture on crop growth and N transformation are modelled synchronically. The land use management routines include modules for fertiliser management, tillage and harvest operation.

All modules are operating on a daily time step. However, hydrologic and solute models are flexible and adaptable in case input data are available in a higher temporal resolution. The model uses a fully distributed modelling approach which allows flexible spatial simulation of hydrologic and solute components in terms of spatial scales and distribution.

Modelling entities for this study were derived according to the ‘Hydrological Response Units’ (HRU) concept extended with a topological routing scheme which allows water and solute transport modelling between RUs based on their topographical location .

Simulation outputs are derived for each of the RUs, or aggregated for chosen parts of a catchment, subcatchments and/or different timescales (e.g., daily, monthly, and annual). These outputs include all components of the water and solute balance as well as simulated time series data like discharge, nutrient concentration or nutrient loads.

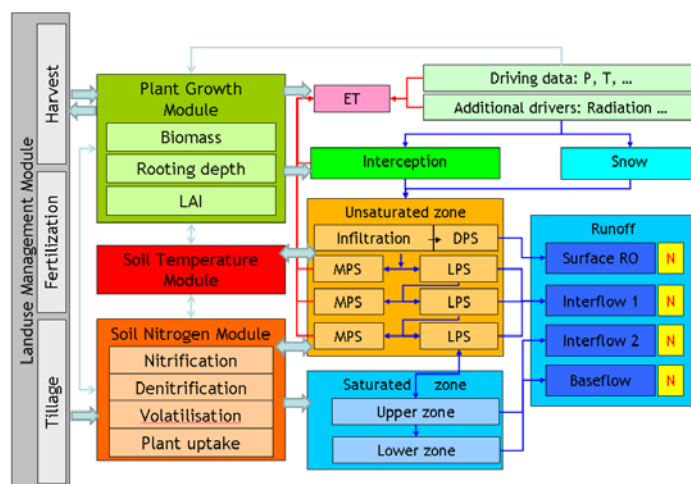


Figure 1. Conceptual hydrologic and solute components of J2000 and J2000-S modules coupled with land use management

2.2. Sensitivity Analysis

Sensitivity analysis of model parameters is used to quantify the impact of single parameters on the model result. Thus, it allows identifying those parameters which should be preferentially considered during a model optimization procedure (Kirkby *et al.* 1993), but also those having minor influence on model results and therefore are set to a constant value (Jansen and Heuberger 1995). Additionally, a sensitivity analysis can be used to identify potential parameter interactions (Schröder 2000) which is important during model calibration because such interactions can increase the uncertainty in finding best parameter sets (Gaume *et al.* 1998). In the literature various methods for analysing parameter sensitivity are discussed which can roughly be distributed into single-parameter and multi-parameter approaches.

The classical single-parameter sensitivity analysis investigates the influence of only one parameter (Anderson and Burt 1995) by changing its value to some defined amount (e.g., $\pm 10\%$) and quantifying the change of the model response. The advantage of this method is that it is fairly quick as it needs only a very limited number of model runs. The disadvantage is that only a very limited amount of the feasible parameter range is tested and that potential parameter interactions cannot be detected.

The multi-parameter sensitivity analysis, often called generalized sensitivity analysis, estimates the impact of a number of parameters contemporaneously. Here, feasible parameter ranges and parameter distribution within these ranges have to be defined prior to the analysis. Then, a Monte-Carlo-Analysis (MCA), sometimes combined with a Latin-Hypercube sampling scheme (McKay 1979), is used in most studies to produce a large number of different parameter combinations and to obtain a model response for each of them. These multiple model responses are then analysed to obtain information about the impact single parameters as parts of parameter ensembles have on the model response. The analysis used for this study is an extension of the Regional Sensitivity Analysis (RSA, Spear and Hornberger 1980) proposed by Freer *et al.* (1996) and used in Wagener *et al.* (2001) in a slightly adapted form. The general idea of the RSA is to split the various model samples into good (behavioural) and bad (non-behavioural) populations and to compare their distribution functions in the parameter/objective function space. Freer *et al.* (1996) sorted model realizations according to specific objective functions and grouped them into ten groups of equal size. With this approach they avoided the subjective selection of a threshold value to distinguish behavioural from non-behavioural models. For these ten groups, distribution functions between the parameter values and the cumulative relative frequency of specific objective functions are created. The appearance of the ten distribution functions per parameter and objective function provides information about the parameter sensitivity – in general the more different the distribution functions are the more sensitive a specific parameter is and vice versa. A second indicator in terms of parameter identifiability and sensitivity are scatter plots - often called ‘dotty plots’ - of the parameter values with respect to single objective functions. In such dotty plots more sensitive parameters produce clearer shapes with a fairly narrow optimal range as they control the model quality to a high degree. Parameters with lower sensitivity produce a more random pattern and optimal values are scattered throughout the parameter range because the objective function is dominated by the more sensitive parameters.

3. STUDY AREA

The coastal, humid Duck catchment is located in the northwest of Tasmania (Figure 2). Since nutrient impacts are considered as very high compared to other catchments in Tasmania (DPIWE, 2003), the Duck catchment was chosen for this study. The entire watershed has an area of about 540 km² and is draining into the Duck Bay and subsequently into the Bass Strait, an area of intensive shellfish production. To avoid tidal influences the gauge at the catchment outlet is located 2.8 km towards the inland resulting in an area of about 370 km². This gauged area was used for model simulation. The catchment characteristics have been previously described by Bende-Michl *et al.* (2007); DPIWE (2003) and Richley (1978). The mixed land use is dominated by dairy in the flat areas on alluvial, partly drained soils as well as grazing beef cattle and forestry in the hilly parts of the catchment.

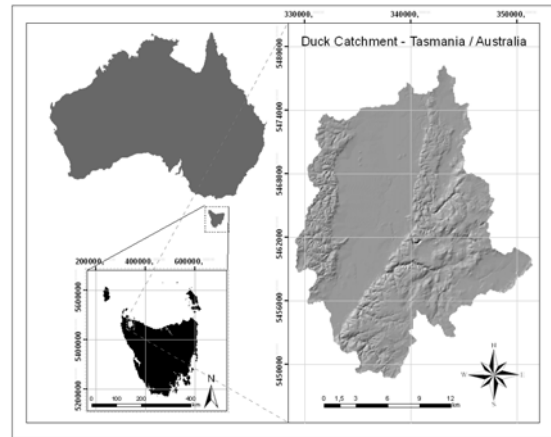


Figure 2. Location of the Duck catchment in Tasmania and entire catchment with the outlet at Scotchtown

Observed nutrient concentrations exceeded the threshold values stated by the ANZECC 2000 guidelines for Tasmanian Rivers (ANZECC 2000). The average observed nitrogen concentrations from the years 1999 to 2006 are 457 ppb ranged from a maximum of 928 ppb to a minimum of 74 ppb (Bende-Michl *et al.* 2007).

4. WATER QUALITY MODELING APPLICATION FOR THE DUCK CATCHMENT

4.1. Data Input and Preprocessing

The climate data used in the model application for the Duck catchment were provided from 14 climate stations from the Australian Bureau of Meteorology (BOM). This included daily time series of precipitation, temperature, sunshine duration, evapotranspiration, relative humidity and atmospheric pressure for a period of 1966 – 2006. The JAMS model was set-up for this period from 1995-2007 as previously being described by Bende-Michl *et al.* (2007). This also included a set of GIS based delineated modelling entities adding up to 6423 HRUs for this application.

4.2. Model Calibration and Validation

The model simulation period included a calibration period from 1995-2002 and a validation period from 2002-2005. The calibration was done manually for only a few model parameters. The long turn-around time per model run prohibited an automatic model optimisation. The results obtained during the calibration were slightly better than those shown here for the validation period. The satisfactory reproduction of the observed versus simulated discharge is shown in Figure 3. The average long-term observed volumetric discharge accounts for 5.01 m³/s in the validation period (DPIW 2003). In contrast the simulated discharge volume was 6.22 m³/s.

The comparison of the observed and simulated runoff for the validation period resulted in a Nash-Sutcliffe efficiency of 0.70, a coefficient of determination (RSQ) of 0.91 and a percent bias of 24%. Despite an overprediction in particular of larger peak flows, the graph show the good agreement of the simulated dynamics with the observed values. Additionally, Figure 3 shows that the model tends to an overestimation of the simulated hydrograph at the beginning of the wet season in autumn (March-May). Three possible reasons can be considered to explain this phenomenon: (i) the initial rainfall might be used to refill dams, (ii) the initial rainfall infiltrates into cracked soils and is not contributing to runoff or (iii) undetected springs out of the karstic system are active. All three rea-

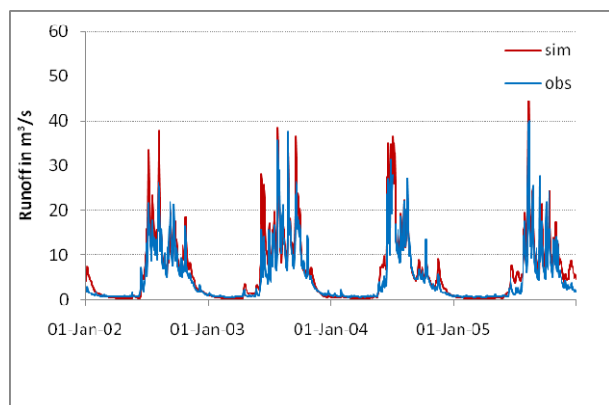


Figure 3. Observed and predicted runoff for the Duck Catchment (Year 2002-2005)

sons could not be addressed with the current model simulation.

The comparison of simulated and observed N-concentrations (2004-2005) shows a reasonable good agreement (Figure 5), showing that the simulated levels fit well with the observed low ranges of nitrogen. The tendency of slight underestimation can partly be explained as a follow up of the slightly overestimated runoff generation. For the dry weather period with stable hydrologic conditions (January to April) nitrogen concentration are strongly under estimated. This might be an indication for groundwater nutrient enrichment as groundwater is the dominant flow path throughout this season which is not covered very well by the model.

4.3. Sensitivity and Uncertainty Analysis

The sensitivity analysis of this study focused on six model parameters which were assumed to strongly affect the nitrogen concentration simulation. To obtain a baseline scenario, the nitrogen concentration curve of the calibrated model was extracted and compared to the model realisations from the MCA. The model parameters used for the sampling were: the denitrification factor (DNF), the rate coefficient for mineralization of the humus active organic nutrient (b_MIN), the nitrate percolation factor (b_NO3), the rate coefficient for mineralization of the fresh organic residue nutrient (b_RSD), nitrogen uptake parameter (b_NDIST) and the nutrient bypass factor (ICF).

The denitrification factor (DNF) determines the rate of bacterial nitrate reduction in the soil. The amount of nitrogen loss by bacterial nitrate reduction depends on temperature, the availability of nitrogen and carbon as well as the on the water saturation of the soil. The two parameters b_MIN and b_RSD control nitrogen turnover rates and therefore the availability of nitrogen in the soil. They determine the rate transfer between the active organic nitrogen pool (b_MIN) and the fresh organic plant residue (b_RSD) and the NO₃-pool. Three parameters are of importance for the distribution within the soil column and therefore nutrient transport via different pathways. The parameter b_NDIST reflects the depth distribution for NO₃ in the soil column to be taken up by plant roots. The parameter b_NO3 allows the rate of mixing for the NO₃ content in surface runoff from the upper soil horizon and the nutrient bypass factor (ICF) determines the amount of nitrate that can bypass the soil matrix, e.g., by preferential flow through macro pores.

For the sensitivity analysis, each of the feasible parameter ranges defined by lower (LB) and upper boundaries (UB) were specified and 2400 uniform random samples were taken. The nitrate concentration model response was compared against the one from the calibrated model and quantified separately with three different objective functions (Nash-Sutcliffe efficiency NSE, percent bias PBIAS and the coefficient of determination RSQ). Table 1 shows the parameter boundaries and the sensitivity of the single parameters in terms of a specific objective function explained later.

Figure 4 shows the scatter plots of single parameters (rows, x-axis) and the values for the three objective functions NSE, PBIAS and RSQ (columns, y-axis) on the left side. Each dot in the single subplots represents one of 2400 model runs obtained from the MCA. The black stars indicate the ten best models in terms of the specific objective function. As clearly illustrated by the scatter plots one highly sensitive parameter, two medium sensitive and three insensitive parameters could be distinguished. The right side shows the cumulative distribution functions for the single parameters and the three objective functions of the Regional Sensitivity Analysis (RSA).

Table 1. Parameter boundaries and sensitivity (+ high, - low) of each parameter for the three objective function Nash-Sutcliffe efficiency (NSE), percent bias (PBIAS) and coefficient of determination (RSQ).

Parameter	LB	UB	NSE	PBIAS	RSQ
DNF	0.80	1.00	+	-	+
b_MIN	0.001	0.003	+	-	+
b_NO3	0.00	1.00	+	+	+
b_RSD	0.02	0.10	-	-	-
b_NDIST	1.00	15.00	-	-	+/-
ICF	0.00	1.00	-	-	-

The figure shows the different sensitivity and identifiability of the six parameters in respect to the three objective functions. Parameter DNF shows a medium to high sensitivity indicated by the clearer shape of the scatter plot. The plot shows that any value greater than a threshold of around 0.975 results in poor model behaviour and poor values for all three objective functions. The parameter DNF can be clearly constrained as for the NSE and roughly constrained for RSQ indicated by the location of the black stars. The RSA functions indicate that 20% of the model runs shows a clearly different behaviour that the other 80%. These are the realisations which produce the poor model performance. The functions of the remaining 80% show a medium diversification indicating the sensitivity of the parameter. Parameters b_MIN and b_NO3 show also a relative distinct shape and a reasonable diversification of the RSA functions for NSE and RSQ, both facts indicating higher sensitivity in terms of the objective functions. PBIAS is influenced by b_MIN and DNF most. The other parameters b_RSD, b_NDIST and ICF are fairly insensitive for the three chosen objective functions.

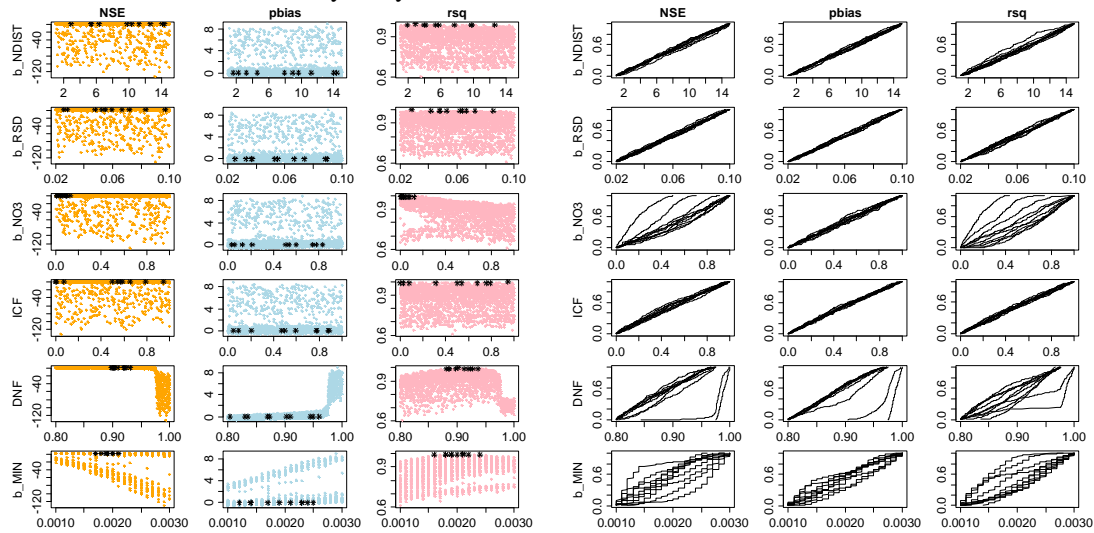


Figure 4. Results of the regional sensitivity analysis of six model parameters based on 2400 random samples.

The runs of the MCA provided not only values of objective functions but also 2400 different model realizations depending on the random parameter samples. These model results were analysed to provide information about the model uncertainty induced by the selected parameters. For this purpose, the 20 % very poor model realisations were removed as they were considered as unrealistic caused by unfeasible values of DNF. From the remaining 1920 model realizations the 5% (Q5) and 95% (Q95) quantile of the N-concentration at the catchment outlet was computed for each time step. The two quantiles were then considered as lower and upper boundaries of a central 90% uncertainty interval and plotted along with the observed N-concentrations in Figure 5.

The results shown in Figure 5 indicate that the model is able to reproduce the measured N-concentrations fairly well, in particular given the fact that observed concentrations are 10 to 20 times lower compared to agriculturally used basins in Europe or the USA. The general model trend shows that the model tends to underpredict the N-concentration during the drier period. This slight underprediction is also illustrated by the comparison of the mean values of the observed (0.44 mg/l) and the simulated N-concentration (0.34 mg/l). The mean values of the quantiles range between 0.18 mg/l (Q5) and 0.55 mg/l (Q95) indicating a reasonable model uncertainty caused by the parameter values.

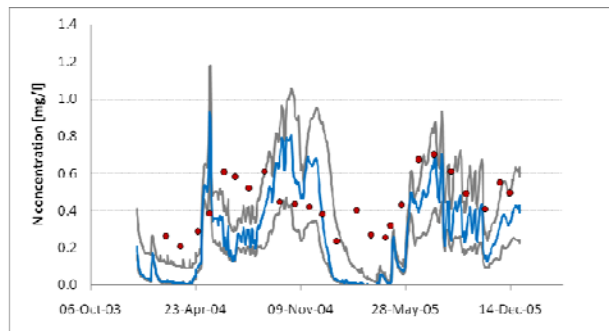


Figure 5. N-concentrations in mg/l for 2004 to 2005. Red dots show observed concentrations whereas the grey lines illustrate the lower and upper boundary of the central 95% confidence interval obtained from 1920 realisations of the Monte-Carlo-Analysis the blue line the N-concentrations from the calibrated model.

5. CONCLUSIONS

The sensitivity and uncertainty analysis carried out for the Tasmanian Duck catchment highlighted the different sensitivity of six parameters addressing the modelling of nitrogen dynamics. The three critical (sensitive) parameters were those directly influencing the availability of nitrate in the catchment and subsequently the simulated nitrate concentration at the catchment outlet: the nitrate mixing parameter for surface runoff, the rate coefficient for the nitrogen turnover controlling the active organic soils, and the nitrate pool. The latter is of importance for the Tasmanian test catchment since a high amount of manure return is adding up to the rapid decaying organic soil nitrogen pool. Additionally, the sensitivity analysis revealed that parameter values of DNF beyond a specific threshold seem to have a very high negative impact on the model results. This might be caused by an inconsistency in the model structure and the underlying model equation. This deficit has to be addressed in further studies by a thorough testing of this specific model behaviour. Nevertheless, this study provided important insights into the model structure and process component functioning as well as valuable information about feasible model parameter ranges for the Tasmanian conditions.

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