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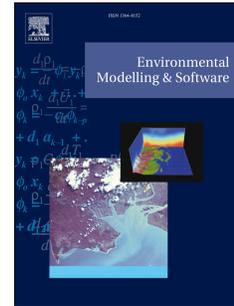
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# Accepted Manuscript

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# Coupling land-use change and hydrologic models for quantification of catchment ecosystem services

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**Abstract.** Representation of land-use and hydrologic interactions in respective models has traditionally been problematic. The use of static land-use in most hydrologic models or that of the use of simple hydrologic proxies in land-use change models call for more integrated approaches. The objective of this study is to assess whether dynamic feedback between land-use change and hydrology can (1) improve model performances, and/or (2) produce a more realistic quantification of ecosystem services. To test this, we coupled a land-use change model and a hydrologic model. First, the land-use change and the hydrologic models were separately developed and calibrated. Then, the two models were dynamically coupled to exchange data at yearly time-steps. The approach is applied to a catchment in South Africa. Performance of coupled models when compared to the uncoupled models were marginal, but the coupled models excelled at the quantification of catchment ecosystem services more robustly.

**Keywords:** model coupling, ecosystem services, integrated modelling, land and water

# 1 Introduction

Land-use and hydrology are strongly interlinked whereby changes in land use affects hydrologic processes including interception, evapotranspiration, infiltration, stream flow and runoff (Costa et al., 2003; Niehoff et al., 2002; Tong and Chen, 2002; Warburton et al., 2012). Similarly, changes in hydrologic processes can influence the distribution and availability of water resources, which in turn can influence processes driving land-use and land cover changes. Changes in hydrologic components, for example, impact parameters associated with land-use suitability for agriculture including soil water balance, leaf area index, vegetation/crop growing seasons, vegetation root depth and root mass distributions (Calder, 1998; DeFries et al., 2004). Modelling the dynamic interactions between these sub-disciplines is an important endeavor that deserves more attention in the environmental modelling community (DeFries and Eshleman, 2004; Wagner et al., 2017). Most modelling practices on interactions of land-use and hydrology using respective models display notable limitations: (1) a static land-use map is used for an entire simulation period in most hydrologic models and modelling practices. Such representation of land-use is problematic because rates and magnitudes of land-use changes are dynamic in practice and the changes can be significant over a modelling period. Apart from biophysical factors such as weather and climate variability, land-use dynamics can also be driven by various social, economic and spatial factors including population, values of commodities, distances from various resources, infrastructures, and services (Lambin et al., 2003; Lambin et al., 2001; Verburg et al., 2004). (2) Hydrologic models are often developed to work only with biophysical inputs such as slope, soil, land use, and weather datasets. This leaves out aspects of socio-economics that contribute to changes in hydrologic processes and water resources directly or indirectly through, for instance, growing population and associated pressures on land-cover and land-use demands. If no socio-economic aspects are considered in hydrologic models, it would necessarily imply that any two catchments whose biophysical input components are equivalent will be assumed to have the same rates of changes and projections irrespective of specific environmental and socio-economic dynamics (e.g. population, density of settlement, in/out-migration, lifestyle, and demands for spatially relevant commodities such as land). (3) Likewise, most land-use change models ignore hydrologic components altogether in their simulations, and those that consider it, take limited proxies of hydrology/water resources using variables, such as average precipitation or distance from water sources, as primary inputs. This results in an oversimplification that ignores all other factors including rainfall intensities, infiltration rates, runoff components, and evapotranspiration, which can influence soil water balance, land suitability and productivity. Ignoring such hydrologic components and discounting water availability in land-use modelling can result in an unconstrained model with regards to potential or actual water resources availability and, thus, can lead to misleading conclusions. (4) On the other hand, even though modelers are aware of the limitations mentioned, incorporating all the depth and breadth of specialized disciplines of hydrology and land-use change into one model can be overly complex.

Integrated modelling methods have been advocated to address, at least partly, the problems mentioned above. Their holistic approach to socio-environmental problem solving in general and in land and water resources management in particular has

been an important attribute of a comprehensive socio-environmental framework (Hamilton et al., 2015; Jakeman et al., 2013; Laniak et al., 2013). In line with this philosophy, an overarching discipline in the water domain, known as socio-hydrology (Sivapalan et al., 2012; Wheater and Gober, 2011), has emerged recently that emphasizes exploration of integrated socio-economic and anthropogenic feedbacks between land-use change and hydrology (Di Baldassarre et al., 2015).

Integrated modelling comes with its own challenges. One of the main challenges is associated with calibration and evaluation mechanisms in integrated subsystems. Changes in variables that used to impact only relatively some part of a subsystem can propagate throughout the whole integrated system (Voinov and Shugart, 2013). A more 'conservative' approach of integrated modelling is often adopted in many interdisciplinary modelling practices where specialized models from various disciplines are calibrated and evaluated independently and exchange data with other models through coupled systems. Model coupling combines specialized models in their entirety instead of relying on simplifications of the specialized models within an integrated framework. Proponents of this approach argue that the coupling approach enables a greater degree of transparency and accuracy in integrated models landscape and watershed models (Robinson et al., 2017; Verburg et al., 2016).

Landscapes provide a number of provisioning and associated ecosystem services (Millennium Ecosystem Assessment, 2005). Agricultural intensification and extensification has enabled substantial increases in provisioning services (e.g. food production) by exploiting available land and water resources, but it has also transformed and degraded natural watersheds and landscapes. To counterbalance the negative effects of intensive agriculture, there is increasing interest in multifunctional landscapes and watersheds for sustainable use natural resources and associated supporting, regulating and cultural ecosystem services (Scherr and McNeely, 2008). Ecosystem services are often evaluated and quantified in association with land and water resources. Grasslands provide ecosystem services in the form of animal feeds/grazing, erosion control, water regulation, soil carbon retention, and biodiversity conservation (Lemaire et al., 2011; White et al., 2000). It is expected that, in the face of climate change and growing demands for agricultural land and productivity, future pressures on grassland ecosystems will intensify (Watkinson and Ormerod, 2001).

The main objective of this study is to evaluate whether dynamic feedback between land-use change and hydrologic models can improve performances of the respective models and/or whether it can produce a more realistic quantification of catchment ecosystem services. We coupled and tested the effect of dynamic feedback between two respective models: SITE (Simulation of Terrestrial Environments) and, SWIM (Soil and Water Integrated Model). The approach is applied to the Thukela catchment (11,326 km<sup>2</sup>) in South Africa as a continuation of our prior experiment on the identification, valuation and mapping of various ecosystem services in the catchment (Yalew et al., 2014). Specifically, this study investigates the effect of model coupling on the sustainability of one of the common ecosystem services of grasslands in the catchment, namely grazing. Quantifying interactions of grassland ecosystem services and water resources in the catchment allows an

## 2 Background and study area

This study is conducted with an aim of supporting an ongoing investigation for better quantification and mapping of grassland ecosystem services in the Thukela catchment, South Africa (AFROMAISON, 2016; Johnston et al., 2014). Besides the identification, valuation and mapping of the various ecosystem services in the case study, a focused analysis and modelling of the interactions of grasslands and water resources with respect to grassland ecosystems services management is a valuable input to decision makers on the ongoing effort to integrated management of natural resources in the catchment (Johnston et al., 2014).

The Thukela catchment is the largest river system of the Thukela district in KwaZulu-Natal province in South Africa (Fig. 1). It is characterized by marked biophysical gradient and diversity of habitat types determined by altitude, slope, climate, topography, and geology. The catchment represents the entire district that is predominantly rural. It is characterized by socio-economic indicators such as low revenue base, poor infrastructure, limited access to services, and low economic base. It had a population of about 670,000 inhabitants in 2011, resulting in a population density of 60 people/ km<sup>2</sup>, with a slightly increasing trend.

Among the most substantial pressures to ecosystems in the study area are intensive livestock grazing and poor land management practices, leading to soil loss and land degradation. On the one hand, the grassland biome, which forms a large and important component of South African vegetation (Scott-Shaw and Schulze, 2013), is fragmenting, impacting the most common grassland ecosystem service, namely grazing. On the other hand, livestock has major economic and social values for the communal farmers in the region and thus grassland ecosystem services will continue to be essential. Beyond its economic benefit, livestock is also used as a sign of prestige in the community (Salomon et al., 2011). High livestock density and poor soil and land management practices, among others, are attributes causing degradation of the grasslands in the Thukela catchment (Scott-Shaw and Schulze, 2013). In addition, increasing competition for demand on arable and urban land use decreases the extent of the grazing land available for livestock. The combined effects lead to unsustainable environmental outcomes with substantial pressure on land and water resources.



### 3.1 The hydrologic model

We used the SWIM model (Krysanova et al., 1998) for hydrologic modelling of the catchment. SWIM is an open-source model used to simulate eco-hydrologic processes such as runoff generation, nutrient and carbon cycling, river discharge, plant growth, crop/biomass yields and erosion (Krysanova and Wechsung, 2000). It can simulate agricultural management, feedbacks of climate and land-use changes as well as dynamic vegetation growth processes (Krysanova et al., 1998). SWIM takes meteorological, topographic, soil and land-use datasets as inputs. It operates at a daily time-step and uses a three-level spatial discretization scheme: watershed, sub-basin and hydrotopes. Sub-basins are delineated from digital elevation model (DEM) and represent small individual watersheds whereas hydrotopes are small hydrologic units with similar land use, vegetation and soil types (Fig. 2).

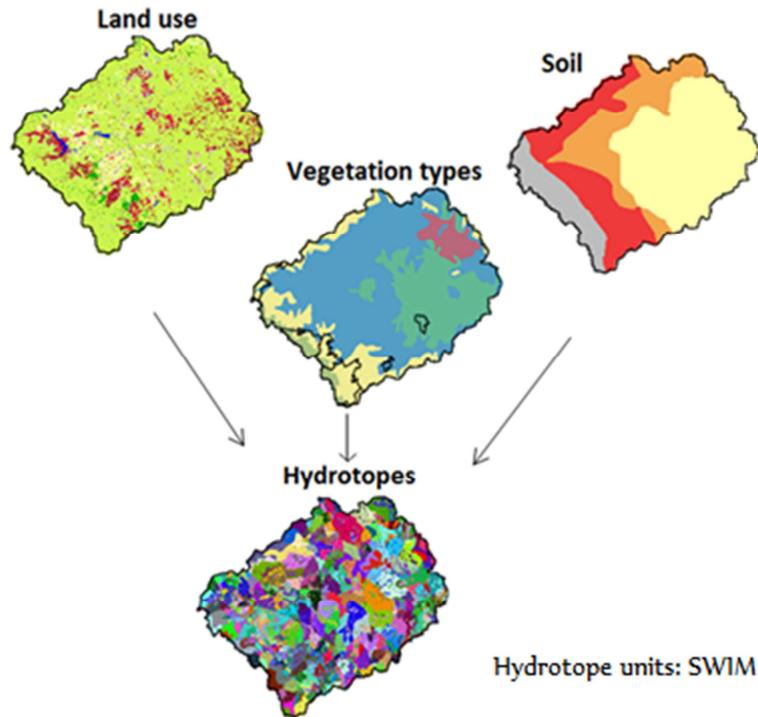


Figure 2. Setup of hydrotope units in SWIM

#### 3.1.1 Inputs and setup

Inputs for the SWIM model include soil, land use, and meteorological data including precipitation, temperature, solar radiation, and relative humidity. Soil information was derived from the Harmonized World Soil Database (FAO et al., 2012). Meteorological information was taken from the Water and Global Change (WATCH) project (Weedon et al., 2010). Streamflow data was derived from the Global Runoff Data Centre (GRDC, 2013), and from the South African Department of

Water Affairs (DWA, 2013). Hydrology in SWIM is governed by the water balance equation that is calculated at the hydrotope level, Eq. (1).

$$\Delta S_t = S_t - S_{t-1} \quad (1)$$

where  $\Delta S_t$  is given by the difference in the amount of water stored in the soil between time  $t$ , and time  $t - 1$ .

The biomass produced after each hydrologic year by SWIM is used as input by SITE. For that, a specific number of potential heat units required for maturity has to be defined for each vegetation/crop type in SWIM. The computation of biomass accumulation follows the approach of Monteith et al. (1977). Photosynthetic active radiation ( $P_{AR}$ ) estimated from input solar radiation and leaf area index (LAI) is used to calculate potential biomass accumulation, Eq. (2).

$$\Delta B_p = B_E * P_{AR} \quad (2)$$

where  $B_E$  is a crop specific factor converting energy to biomass.  $\Delta B_p$  is then reduced to get the daily actual biomass increase, Eq. (3).

$$\Delta B = \Delta B_p * R_{EGF} \quad (3)$$

$R_{EGF}$  is a growth regulating factor constraining biomass accumulation due to plant stress. These stresses include water, temperature, Nitrogen (N) and Phosphorus (P), calculated separately. The leaf area index (LAI), which is defined as the one-sided green leaf area per unit ground surface area, is then estimated by an empirical function of accumulated heat units and above-ground biomass. SWIM, therefore, produces yearly cumulative vegetation biomass (including for grasslands) as a function of these stressors.

### 3.1.2 Model calibration: SWIM

The hydrologic model was calibrated for 1990-1994 and validated for 1995-2000 using flow data at the catchment outlet. A static land-use map of 1990 reclassified from the National Land Cover Data of South Africa (South African Environmental Affairs, 1990) was used as a base and calibration map for the SWIM model. The five year calibration period was defined in such a way that it contains wet, average, and dry years. Parameters including base flow factor, alpha factor for ground water, ground water delay, evaporating fraction of ground water, percolating fraction of shallow ground water, evaporation threshold of ground water, potential evapotranspiration correction factor, routing coefficient both for surface and subsurface flows, correction factor for saturated conductivity, and leaf area index were calibrated manually by visual inspection of discharge plots. Parameter sensitivity analysis initially tested on the model was unable to clearly identify the most notable parameters that earlier researches in the catchment identified to be influential. The most important parameters in the catchment based on previous studies were included in this manual calibration. Performance indicators of the percent bias (PBIAS) (Moriassi et al., 2007) and the Nash-Sutcliffe efficiency (NSE) (Nash and Sutcliffe, 1970) were used for this purpose. PBIAS is an error index describing the average tendency of simulated values to be larger or smaller than observed data (Moriassi et al., 2007) as shown by Eq.(4).

$$PBIAS = \frac{\sum_j(Sim_j - Obs_j)}{\sum_j(Obs_j)} * 100\% \quad (4)$$

where  $Sim_j$  is the simulated and  $Obs_j$  is the observed value at time-step  $j$ , respectively.

In this case it is given in percent, and the optimal value is  $PBIAS = 0\%$ , whereas model accuracy gets worse the greater the deviation from zero. Positive values indicate model overestimation bias and negative values indicate model underestimation bias. Nash-Sutcliffe efficiency (NSE) is a dimensionless model performance measure commonly used in hydrologic modelling. It is the ratio of residual variance to variance in observations, Eq. (5).

$$NSE = 1 - \frac{\sum_j(Sim_j - Obs_j)^2}{\sum_j(Obs_j - Obs_{mean})^2} \quad (5)$$

where  $Obs_{mean}$  is the mean of observations over the analysis's time period.

Model performances are generally considered satisfactory if  $NSE > 0.5$  and  $PBIAS < \pm 25\%$  (Moriassi et al., 2007).

### 3.2 The land-use model

Although still in development addressing methodological and paradigmatic challenges compared to those with established models in hydrology in general, a growing number of land-use change models with varying degree of complexity and design objectives have been made available in the last couple of decades. Questions of interest in this growing field of modelling include whether a particular land-use change model is deterministic or probabilistic (Koomen and Stillwell, 2007), whether it is spatially aggregated or spatially explicit (Schweitzer et al., 2011; Verburg et al., 2004), whether it is agent-based or pixel-based (Agarwal et al., 2002), and whether it is static or dynamic (Veldkamp and Verburg, 2004). Overall, land-use change models vary in degrees of complexity, objective and applicability.

In this study, we used the SITE land-use modelling framework (Schweitzer et al., 2011) to develop a land-use change model for the Thukela catchment. SITE was selected due to its suitability for representing socio-economic as well as biophysical inputs and due to its capability for spatially explicit land-use change simulation. It is a cellular automata based multi-criteria decision analysis framework for simulating land-use conversion based on socio-economic and environmental factors (Schweitzer et al., 2011). It also provides a number of algorithms and tools such as for model evaluation, calibration and visualization. In addition, the model can be easily modified as it allows access to its underlying modelling sequence. SITE comprises of two model domains: the system domain where methods, procedures and essential algorithms for model initialization simulation are programmed, and the application domain where case specific decision rules are implemented.

### 3.2.1 Inputs and setup

The land-use model was developed to simulate from 2000-2010. Input data for SITE included the initial land-use map of 2000 derived from GLC30- a 30m resolution global land cover product (GLC30, 2014; Jun et al., 2014). Land-use maps of 2000 and 2010 derived from this product are used for base and reference maps, respectively, for the land-use simulation model. The maps are reclassified and include land-use categories of water bodies, forest, shrub land, savanna, grassland, wetland, cultivated/cropland, vegetation mosaics (abbreviated as ‘veg\_mosaic’ hereafter), urban settlement and bare land using two other high resolution (15m) local land-use products for the years 2005 and 2008 (Ezemvelo, 2011). Other inputs for the land-use model include data on population, livestock, biomass (average biomass dynamically passed from the hydrologic model at a yearly time-step), protected/reserved areas, computed distances from water, road, and urban centers and slopes derived from digital elevation models (DEMs). The model dynamically allocates land-uses based on projected demands derived by population and livestock for various uses (see section 3.4).

### 3.2.2 Model calibration: SITE

Land-use models are often calibrated based on a number of parameters. SITE comes with the GALib genetic algorithm library (Wall, 1996), which is used for the purpose of auto-calibration. In this study, the GALib algorithm was used for calibration land-use change related parameters including land-use suitability factor, coefficient of protection of protected area, cover factor, and management/conservation factors. Starting simulation with the base map of 2000, the simulated map for the year 2010 is compared with the reference map for the same year using the Quantity and Allocation Disagreement measures (Pontius and Millones, 2011). Quantity disagreement (QD) is the difference between two maps due to an imperfect match in overall proportions of all mapped land-use categories whereas allocation disagreement (AD) is the difference between two maps due to an imperfect match between the spatial allocation of all mapped land-use categories (Pontius and Millones, 2011). This measure summarizes confusion or error matrix derived from the spatial comparison between the simulated and the reference maps using a pixel as a spatial assessment unit. The measure, thus, indicates the percentage of correctly classified pixels using equations (6) and (7).

$$AD = \frac{\sum(2 * \min(\frac{n_{+i}}{n}, \frac{n_{i+}}{n}))}{2} * 100 \quad (6)$$

$$QD = \frac{\sum |\frac{n_{+i}}{n} - \frac{n_{i+}}{n}|}{2} * 100 \quad (7)$$

where QD=quantity disagreement; AD=allocation disagreement;  $n_{ii}$  = diagonal matrix elements;  $n$  = total number of considered pixels; and  $n_{+i}$  and  $n_{i+}$  = marginal sum of the columns and marginal sum of the rows in the error matrix, respectively.

Unfortunately, no unique threshold exists in the literature that defines the acceptable values of accuracy for map comparisons in general. Although not particularly for QD and AD, Landis and Koch (1977) suggested agreement ranges of map comparison results into three groups: agreement value greater than 0.8 (80%) represents strong agreement; agreement value between 0.4 (40%) and 0.8 (80%) represent moderate agreement; and agreement value less than 0.4 (40%) represents poor agreement between two maps. We used this rough guide to evaluate the performance comparison between the simulated and the reference land-use maps.

### **3.3 Demands for land use**

In relation to land-use demand projection for the land-use model, past trends of population, livestock, settlement, and land-use change are used. The population growth rate in the Thukela district is 0.17%/year (Lehohla, 2012). Increased livestock population in the rural community in this district, besides its commercial value, is a sign of more wealth and respect (Johnston et al., 2014; Salomon, 2006). The annual livestock growth rate for South Africa between 1990 and 2000 was reported to be 0.2%/year (FAO, 2004, 2005). For the land-use change model simulation, we assumed the same annual livestock growth rate to continue to 2010. Therefore, annual population growth rate of 0.17% and livestock growth rate 0.2% together with their associated demands for various land uses and land-use related services are used for the model simulation.

### **3.4 Ecosystem services assessment**

Grasslands provide ecosystem services in the form of, for instance, grazing, erosion control, water regulation, soil carbon retention, and biodiversity conservation (Lemaire et al., 2011; White et al., 2000). In this study, we used a single ecosystem service associated with the grassland land-use type, namely, grazing, to test the effects of dynamic feedback between hydrology and land-use for ecosystem services assessment. Thus, we did not try to analyze comprehensive ecosystem service provisions by all land-use types, and neither did we try to analyze all ecosystem services provided by the grassland in the catchment.

We used the concept of carrying capacity (Cowlshaw, 1969) to characterize the sustainability of grazing. Carrying capacity, with respect to livestock grazing, refers to the number of grazing animals a landscape is able to support without depleting rangeland vegetation or soil resources. It is defined as the area of land at a given time that is able to provide for a certain number of animals, expressed as animal-units per area (de Leeuw and Tothill, 1990; Tainton, 1999 ; Tainton et al., 1980). An animal unit (AU) is defined to be equivalent to a 450kg cow (Leistriz et al., 1992). One AU is assumed to consume 12kg of

forage dry matter (biomass) per day, or 4.38 metric tons per year (Scarnecchia, 1985). Under sustainable management objectives, the actual amount of forage available for livestock grazing must be less than total biomass produced from the grassland (Fernández-Giménez and Swift, 2003). An adjustment for allowable use must be incorporated into the calculation to ensure that some un-grazed residual biomass is maintained to protect soil and vegetation resources (Kemp et al., 2000). With sustainable grassland ecosystems management in mind, the recommended minimum grazing capacity for the Thukela district is 0.5 AU/ha (Spehn et al., 2006). This would imply that at least a minimum of 6kg of dry matter per hectare per day (0.5\*12kg/day), equivalent to 2.19 metric tons per hectare per year, should be available as residual biomass to maintain the sustainability of grazing ecosystem service of the grassland. Lower amounts imply overgrazing, soil erosion and/or land degradation on the catchment landscape that are deemed unsuitable for grazing. On studying factors influencing grassland grazing capacity, Holechek et al. (1995) suggest that distance from water and slope are also important considerations (see Tables 1 and 2).

**Table 1. Reductions in grazing capacity with distance from water.** Source: Holechek et al. (1995)

Distance from Water (km)	Reduction in Grazing Capacity (%)
0-1.6	0
1.6-3.2	50
>3.2	100

**Table 2. Reductions in grazing capacity for different slopes.** Source: Holechek et al. (1995)

Slope (%)	Reduction in Grazing Capacity (%)
0-10	0
11-30	30
31-60	60
>60	100

These distance and slope factors state that any amount of grassland biome outside or beyond the suggested upper limits of the ranges in these tables would imply that the resources are simply unreachable for livestock grazing. Integrating the above, the grazing capacity of a grassland ecosystem can be represented by Eq. (6):

$$G_c = B_y - \left( B_y * \frac{S_c G_c}{100} + B_y * \frac{D_c G_c}{100} \right) - B_{min} \quad (6)$$

where  $G_c$ =grazing capacity (in metric tons) per hectare per year;  $B_y$ =yearly grassland biomass (metric tons) per hectare per year;  $S_c G_c$ =percentage reduction in grazing capacity for the respective slope class;  $D_c G_c$ =percentage reduction in grazing capacity for the respective distance from water class; and  $B_{min}$ =minimum biomass to be maintained per hectare per year for a sustainable grassland ecosystem, i.e., 0.5AU/ha, which is equivalent to 2.19 metric tons/ha per year.

This equation (Eq. 6) is implemented on the land-use model for assessing the grazing capacity of the grassland using biomass produced and forwarded from SWIM at each time-step. Note that the grazing capacity  $G_c$  calculation produces only available biomass for livestock in terms of metric tons. This value can be divided by 2.19 to get the potential number of livestock the biomass can support. On the other hand, this potential livestock support can be compared with the density of livestock on the ground, whereby dynamic reduction of livestock may be implemented when enough forage is not available. However, given the high level (low resolution) spatial data about livestock density, we rather resorted to demonstrating the potential biomass capacity that can serve increasing livestock numbers (with annual rate of growth) on existing spatial units. So the assumption is that livestock is a dynamic component in the model (as it grows in number, its forage requirement increases too), but it is not dynamic in terms of, for example, response to shortage in forage supply.

### 3.5 Model coupling

While a universal definition for integrated modelling in environmental sciences is still evolving, it is generally accepted that it brings knowledge from two or more (sub-) domains to a common framework for interdisciplinary analysis. Integrated modelling involves linking of disciplines, processes, and/or scales depending on objective of the integration and data availability (Kelly et al., 2013). Model integration is often carried out through coupling of two or more specialized models from different (sub-) disciplines. Recently, a desire to integrate land-use change and hydrologic models has evolved (Karlsson et al., 2016; McColl and Aggett, 2007; Monier et al., 2016; Narasimhan et al., 2017). The benefit of such coupling is that watershed planners can examine the present and future characteristic of a specific watershed through analysing effects of land-use change on water resources and vice-versa in an integrated and holistic manner.

#### 3.5.1 Conceptual framework for the coupling

The conceptual framework of the coupling starts with development, calibration and evaluation of two separate land-use change (SITE) and hydrologic (SWIM) models independently. The two independent models are then coupled to exchange data between them dynamically. As shown in Fig. 3, the SWIM model, which quantifies water availability for crop/vegetation growth, produces biomass for the land-use model (SITE). The land-use model determines (based on land-use suitability for various purposes and land-use demands) the land-use pattern that, together with the biomass output from SWIM, is used to estimate ecosystem services. Feedbacks from these services inform adaptation policies or further scenarios. Socio-economic, climatic and management scenarios are used as inputs on both models (Fig. 3).

For the hydrologic model, land-use map is provided dynamically from the SITE land-use change model. SWIM estimates surface runoff as a non-linear function of precipitation and a retention coefficient, which depends on soil water balance, land-use and soil type - a modification of the Soil Conservation Service Curve Number (SCS-CV) method (Krysanova and Wechsung, 2000; Mishra and Singh, 2013). Land-use is dynamically imported to SWIM from the land-use model at the end of each year. Thus, changes in land-use (vegetation covers) produced using SITE affect curve number (CV) and leaf area index (LAI) parameters in the SWIM model, thereby influencing water balance components including evapotranspiration, infiltration, and surface runoff.

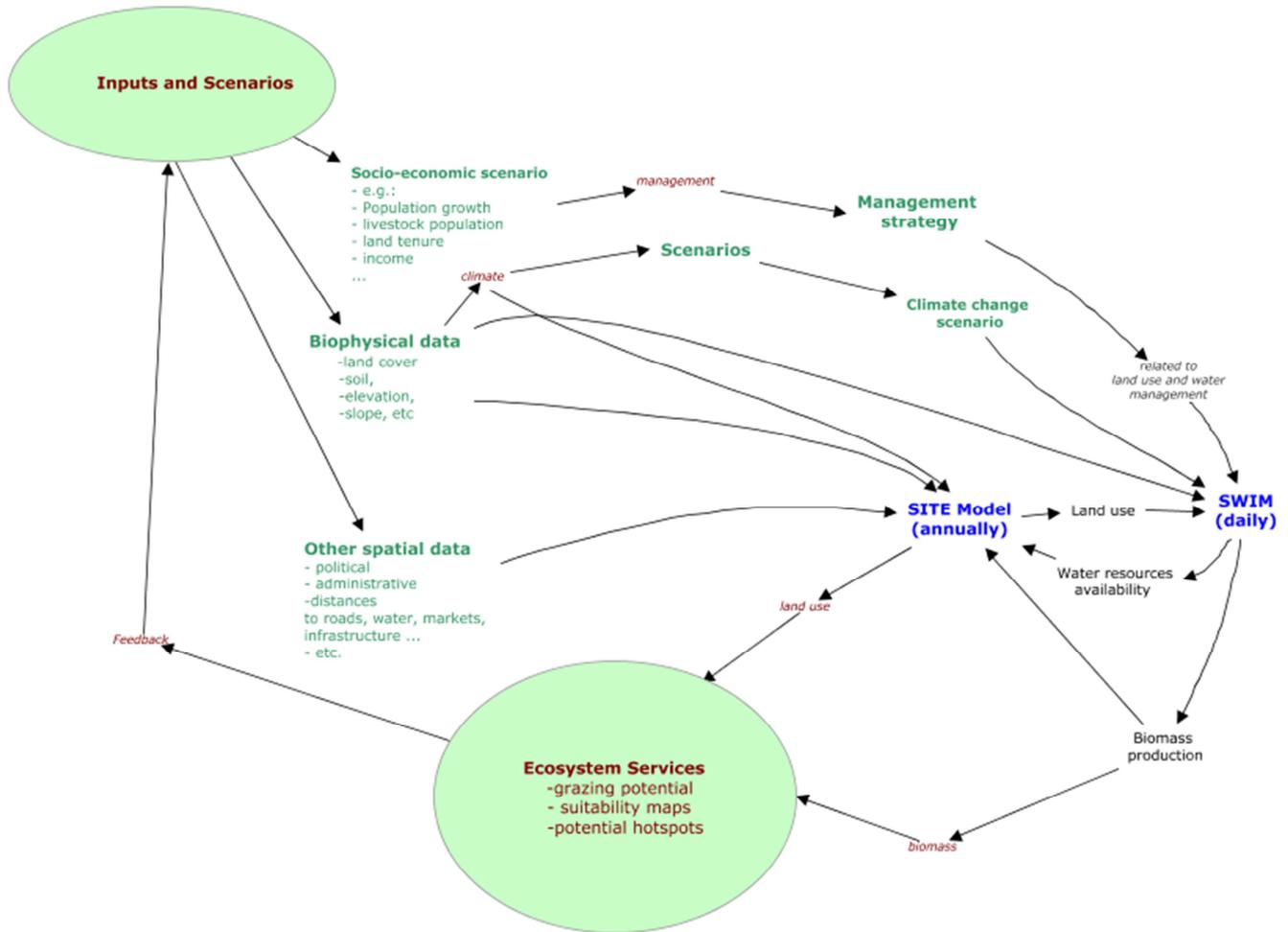


Figure 3. The model coupling schema.

In the land-use model, changes in land-use are determined following two procedures. First, land-use suitability template/map is produced based on soil type, soil texture, elevation, slope, and proximity from various resources and infrastructures, including water bodies, roads, and markets/urban centers. These factors are computed using multi-criteria analysis methods

implemented in the suitability module in SITE. Then, based on the projected demand (associated with population and livestock growth rates) for the various land-uses, land-use is allocated on the template/suitability map. Both the uncoupled and the coupled models include these factors in their simulation of the land-use changes. The coupled model incorporates an additional factor, soil water balance, for computing land-use suitability. Soil water balance is dynamically imported from the hydrologic model. Thus, although some of these land-use suitability factors remain constant during the entire simulation period (such as elevation, slope, soil type, and soil texture, for example) others, including soil water balance, change dynamically. This dynamic continues until the end of the simulation period. In the meantime, the grassland's biomass (evaluated using the hydrologic model) and its potential for sustainable grazing ecosystem service are computed from the results of the coupling. Thus, soil water balance and aboveground biomass imported from the hydrologic model are used for computation of land-use suitability and for quantification of the grazing ecosystem service, respectively.

### **3.5.2 Technical details of the coupling**

Like model integration, model coupling may mean different things for different people. Depending on the level and or type of interaction between participating models, several forms/definitions of coupling are commonly reported in the literature. Among this, loose, tight, and embedded coupling (Bhatt et al., 2014; Brandmeyer and Karimi, 2000) is one. Loose coupling involves exchange of results between two or more models with no need for modification within the participating models. No shared interface exists for the data exchange and thus participating models do not need to run in parallel (Bhatt et al., 2014). Tight coupling involves common interface or controlling unit and shared database for data exchange. Embedded coupling involves the merging (full integration) of processes and modules between participating models in a way that intra-model modification is possible in addition to shared database and a common user interface (Bhatt et al., 2014; Brandmeyer and Karimi, 2000). Other forms/definitions of model coupling include simultaneous, alternating iterative, or externally coupling (Becker and Burzel, 2016), and code level or interface level coupling (Butts et al., 2014). In this study, we followed the first form of coupling (loose, tight, and, embedded), and developed a tight coupling between SWIM and SITE using the general framework presented earlier. This form of coupling enables each of the two models to execute at a commonly defined time-step, which is one hydrologic year (October-September), using a common control script (interface) and a shared database (Fig. 4).

The execution of the coupled models begins by initiating SWIM, using the control script, to run with the base land-use map input of year 2000. [Note that land-use map from 2000 is used as input to the hydrologic model for 2001, thus, the land-use from the end of the previous year is actually used as input to the hydrologic model in the beginning of the current year.] At the end of every yearly simulation, it modifies a log file to signal SITE to continue running using the results of SWIM.

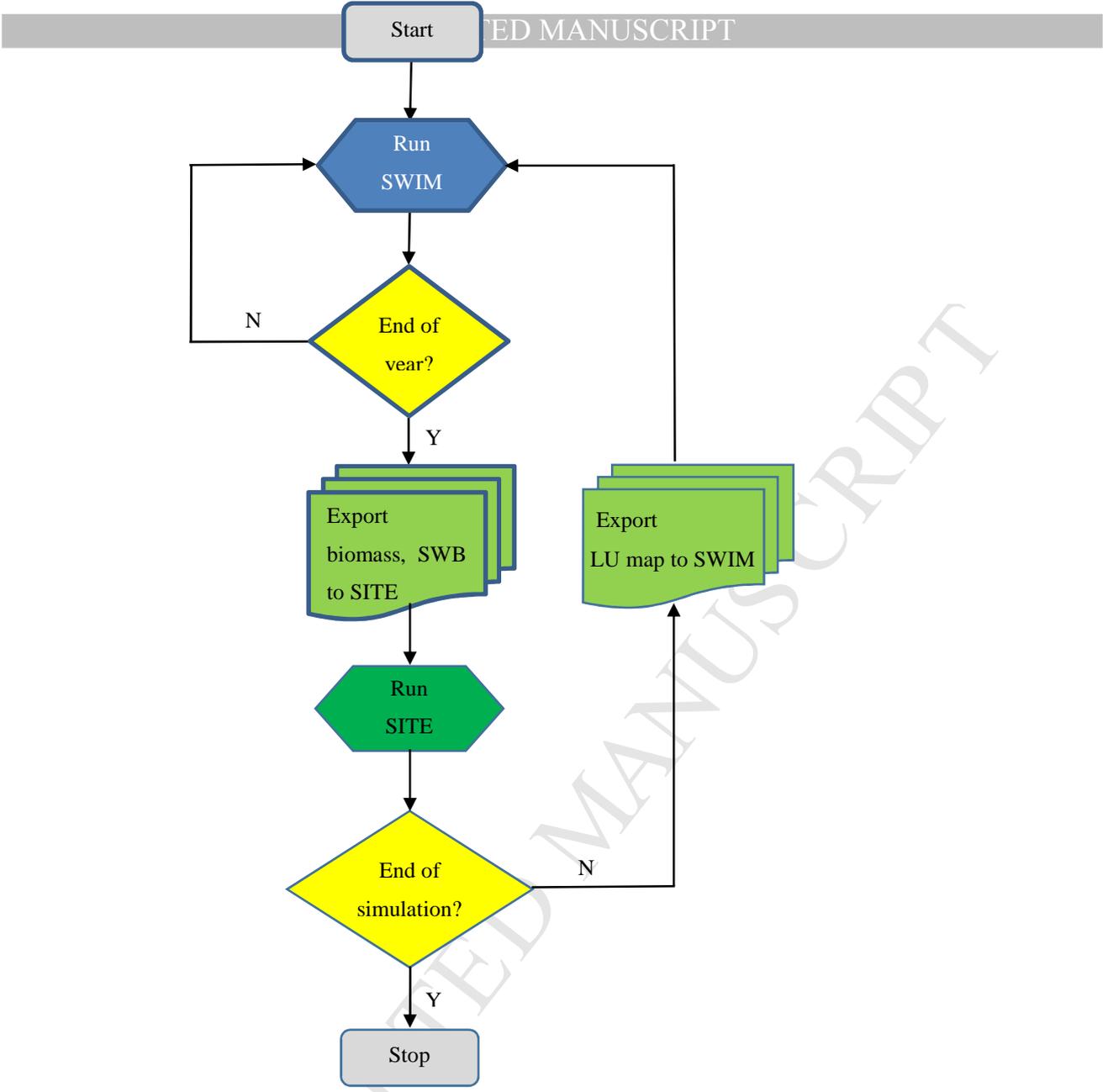


Figure 4. The Model coupling execution flowchart. Note that N is used for ‘no’ and Y is used for ‘yes’.

SITE executes its routine using these results for one time-step (1 yearly simulation) and signals SWIM to continue with its simulation. This way, the *Execute-Signal-Wait-Execute* cycle continues until both models come to the end of the defined simulation period for both. Output of every time-step from one model is used as an input to the other model for the next time-step (Fig. 4).

Internal time-steps setup for each of the models are different: for the land-use model, one time-step is (one year). Since the land-use model operates on a yearly time-step and the coupling data exchange is set to be at yearly time-step, the land-use model's 'internal' and 'external' simulation time-steps are both set at 1. Thus, output from the land-use model is passed to the hydrologic model at the end of each land-use simulation time-step. On the other hand, the hydrologic model operates on a daily basis, and thus has to use a single land-use map for 365 'internal' simulations. Land-use map of the year 2000, for instance, is used as input for the next 365 simulation time-steps (2001) in the hydrologic model. This tight coupling is handled with an external control script, 'coupler.py', that triggers and control the execution process in both models. Thus, after each 'external' simulation time-step, the two models read the execution status parameter in a parameter file, 'param.ini', from a shared database on whether to proceed with simulating or to wait for the other model to complete its time-step. This continues until both the land-use and the hydrologic models finish the simulation step that is defined in the same parameter file, 'param.ini'.

### **Software and scripts**

In total, two existing and three newly developed software programs/scripts are used. The existing models are modified to facilitate the coupling and data exchange.

- **SWIM:** the source code of the FORTRAN based SWIM model was slightly modified for this coupling. Control routines to read/write model execution status, and recursively check for end of simulation step of the model so as to either proceed or wait, by reading from and writing to a commonly accessible file, are implemented in the main ('mainpro.f90') module of the SWIM model. Furthermore, after the first year of simulation, the grazing module in SWIM was modified to compute at the beginning of each new simulation time-step (after the whole grassland biomass has been forwarded to SITE) instead of at the end of each simulation time-step. This is done to facilitate full accounting of the grassland's carrying capacity in the land-use model before any reduction/grazing/regrowth module is applied in SWIM. Since the objective of the ecosystem services quantification is to assess the total sustainably graze-able grassland potential for livestock, the total grassland biomass is passed to the land-use model before reductions due to grazing.

- **SITE:** SITE was used for simulating land-use change and for implementing computation logics that quantify the grassland's potential for sustainable livestock grazing. The main application script in SITE has two functions: the Initialize() and SimulationStep() required by the system domain. The earlier initializes global variables, spatial references and initial grid-cell values. The 'SimulationStep()' function entails tasks to perform at each step of the land-use simulation. The functions to check model execution status, to import biomass and export land-use to/from the shared 'Exchange' data folder(Fig. 4) are implemented in the 'SimulationStep()' function.
- **Ascii2Swim.py:** This python script was written to convert ASCII based grid cell land-use values from SITE and to recreate SWIM hydrotopes at each time-step based on these land-use values. It is discussed earlier that hydrotopes are dependent, among others, on land-use values. Whenever a new land-use map is imported to SWIM at each time-step, the hydrotopes inherently change with it. This script uses the GRASS GIS APIs (Application Programming Interfaces), which are functions for GIS processing in GRASS, for reclassification of hydrotopes and matching SWIM's sub-basins arrangement at each time-step.
- **Swim2Ascii.py:** This script was written to convert SWIM model outputs to an ASCII grid format for use by SITE. It uses GRASS API functions for the conversions at each time-step. Yearly average biomass values produced with SWIM are exported to the exchange folder in this format whereby SITE loads them for its own computations at each time-step.
- **Coupler.py:** This was written to initiate parallel executions of SITE and SWIM, and manage execution processes, irregularities (such as missing input files, delayed response) or errors during execution of the coupled models. It lets the two models run in parallel and proceed with their own input, processing and output unless irregularities/errors in execution are reported.

It is to be noted that only newly developed scripts or modified models that are related to the coupling are listed here. Other dependency tools (such as pyWin, wxWidgets) and pre-processing tools such as GRASS and ArcGIS are used as well.

### ***Operating environment***

Although the individual models can run on Linux operating systems, the coupled models are developed and tested in a Windows environment only. Specifically, windows 7, 64 bit machines are used. The Photran integrated development environment (IDE), based on Eclipse and CDT (C/C++ development tooling), is used for compiling the FORTRAN based modified SWIM code on Eclipse Luna (2016).

## 4 Results

Results corresponding to land-use change and hydrologic components are analyzed both with and without the coupling of the two respective models. Furthermore, the grassland's potential for sustainable grazing ecosystem service and future scenarios are assessed. The results of this assessment are presented in the following subsections.

### 4.1 Hydrologic changes

The uncoupled SWIM model was calibrated for 1990-1994 and evaluated for 1995-2000 (see Table 3 for calibration parameters). Performance measures show NSE values of 0.58 and 0.53, and PBIAS values of -0.17 and -0.21 for the calibration and evaluation periods of the model, respectively (see Fig. 5 and Table 4).

Table 3. Calibrated model parameters and their final values

Parameters*	<i>ecal</i>	<i>thc</i>	<i>roc2</i>	<i>roc4</i>	<i>bff</i>	<i>sccor</i>	<i>abf</i>	<i>delay</i>	<i>revapc</i>	<i>rchrgc</i>	<i>revapmn</i>
Initial values	0.21	0.8	0.5	0.67	0	1.21	0.17	250	0.36	0.1	0.5
Final values	0.53	1.0	0	0.51	1	1.33	0.1	100	0.21	0.04	0

\**ecal*->correction factor for potential evapotranspiration; *thc* ->correction factor for sky emissivity-affects potential evapotranspiration; *roc2* ->routing coefficient -storage time constant of surface flow; *roc4* ->routing coefficient -storage time constant of subsurface flow; *sccor* ->correction factor for saturated conductivity; *bff* ->baseflow factor; *abf* ->alpha factor for groundwater; *delay*->groundwater delay (days); *revapc* ->fraction of groundwater recharge that evaporates; *rchrgc* ->fraction of shallow groundwater that percolates to deep; *revapmn*->threshold of groundwater storage before evaporation can start (mm).

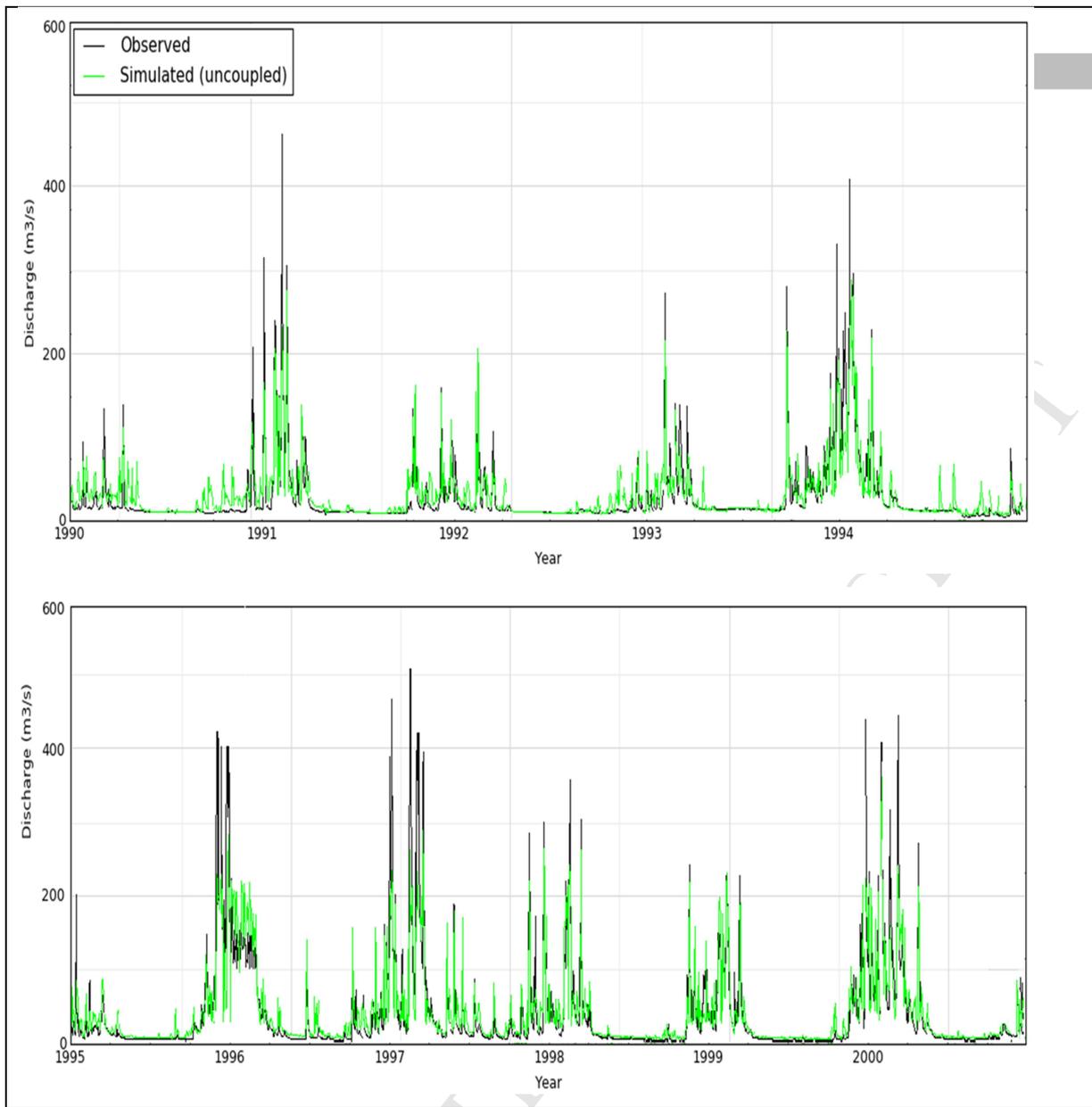


Figure 5. Calibration and validation of the uncoupled hydrologic model

Table 4. Coupled vs. uncoupled SWIM model performance against observed streamflow

Model	Setup	ACCEPTED MANUSCRIPT Calibration (1990-1994)		Validation (1995-2000)		Validation (2001-2010)	
		NSE	PBIAS	NSE	PBIAS	NSE	PBIAS
		SWIM	Uncoupled	0.58	-0.17	0.53	-0.21
	Coupled					0.54	-0.19

Then, SWIM was run from 2001 to 2010 both in coupled and uncoupled mode. Both the coupled and the uncoupled models are re-evaluated against the observed data from 2001-2010 (Fig. 6 and 7). The uncoupled SWIM model showed performance values of 0.52 and -0.22 for NSE and PBIAS measurements, respectively. The coupled hydrologic model showed values of 0.54 and -0.19 for NSE and PBIAS, respectively. Note that SWIM was not re-calibrated for 2001-2010; the simulated dataset is simply re-evaluated against the observed dataset in terms of NSE and PBIAS measures.

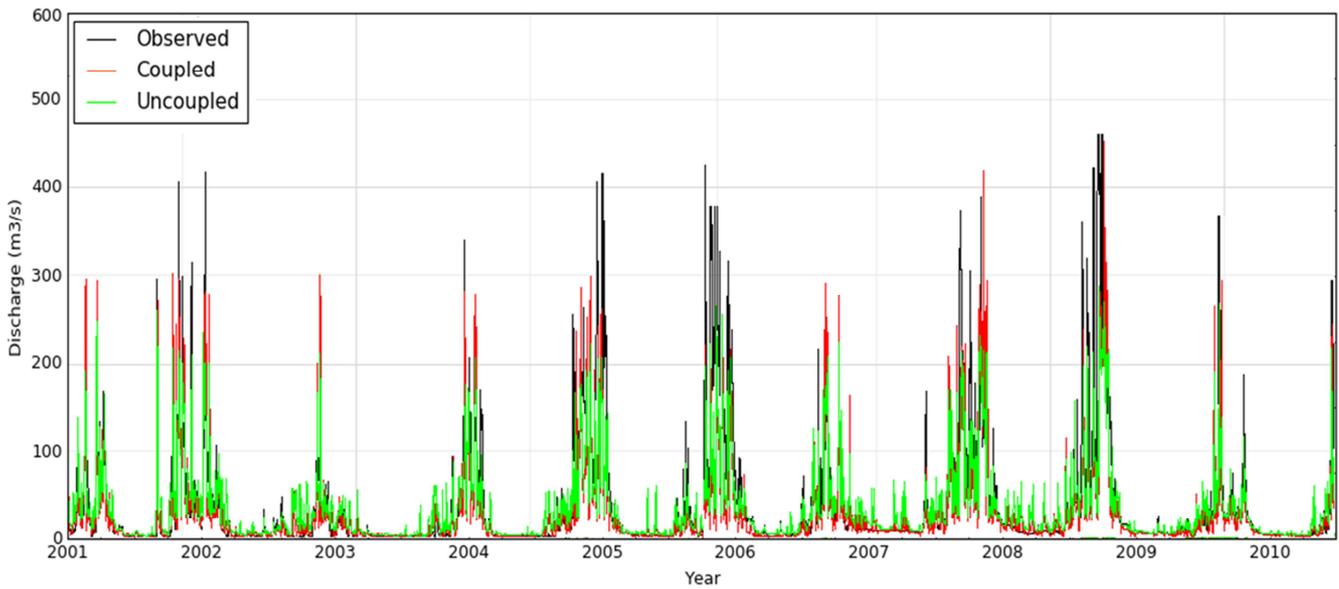
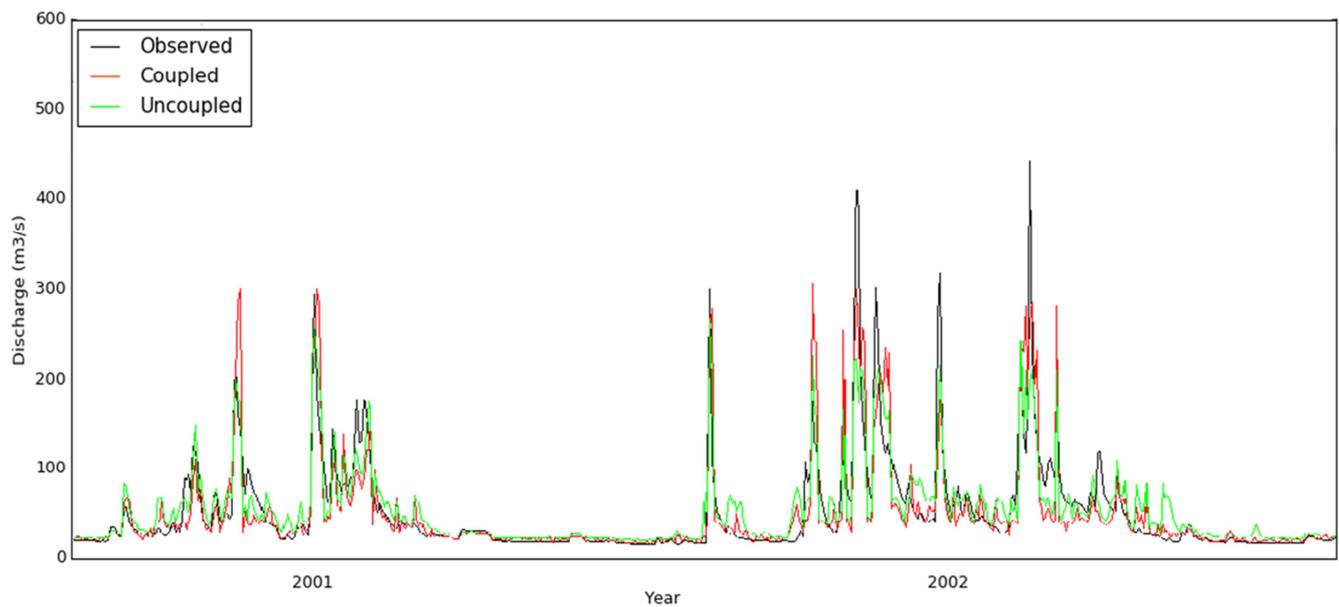


Figure 6. Comparison of coupled, uncoupled and observed flow 2001-2010



**Figure 7. A closer look of the coupled and uncoupled flow simulations (2001-2002)**

Table 5. Overall average comparison with observed flow (% difference) from 2001-2010.

Flow components*	Model	
	Coupled model	Uncoupled model
High-flow	-18.7	-26.5
Average-flow	-5.2	-7.0
Low-flow	-6.3	-4.5

\*N.B. High-flow is represented by flows of 200 m<sup>3</sup>/s and above, average-flow is represented by flows from 30 m<sup>3</sup>/s to 200 m<sup>3</sup>/s, and low-flow is represented by flows below 30 m<sup>3</sup>/s, all assumed from observation of the streamflow hydrograph.

Overall average flow comparison in terms of percentage difference with the observation is shown in table 5. For this analysis, the stream-flow components were separated in terms of high-flow, average-flow and low-flow regimes/seasons via visual examination of the streamflow hydrograph in Fig. 7. Accordingly, flows above 200 m<sup>3</sup>/s are assumed as high-flows, and those in between 30 m<sup>3</sup>/s and 200 m<sup>3</sup>/s are assumed to be average-flows. Flows less than 30 m<sup>3</sup>/s are assumed to be low-flows for this analysis. From Table 5, we can see that the result of the simulated flow from the uncoupled model has a larger percentage difference against the observed flow on high-flow seasons compared with the result from the coupled model. Results of the average-flow and the low-flow seasons from both the uncoupled and the coupled models are comparable, with a slight advantage of the uncoupled on the low-flows and the coupled on the average-flows.

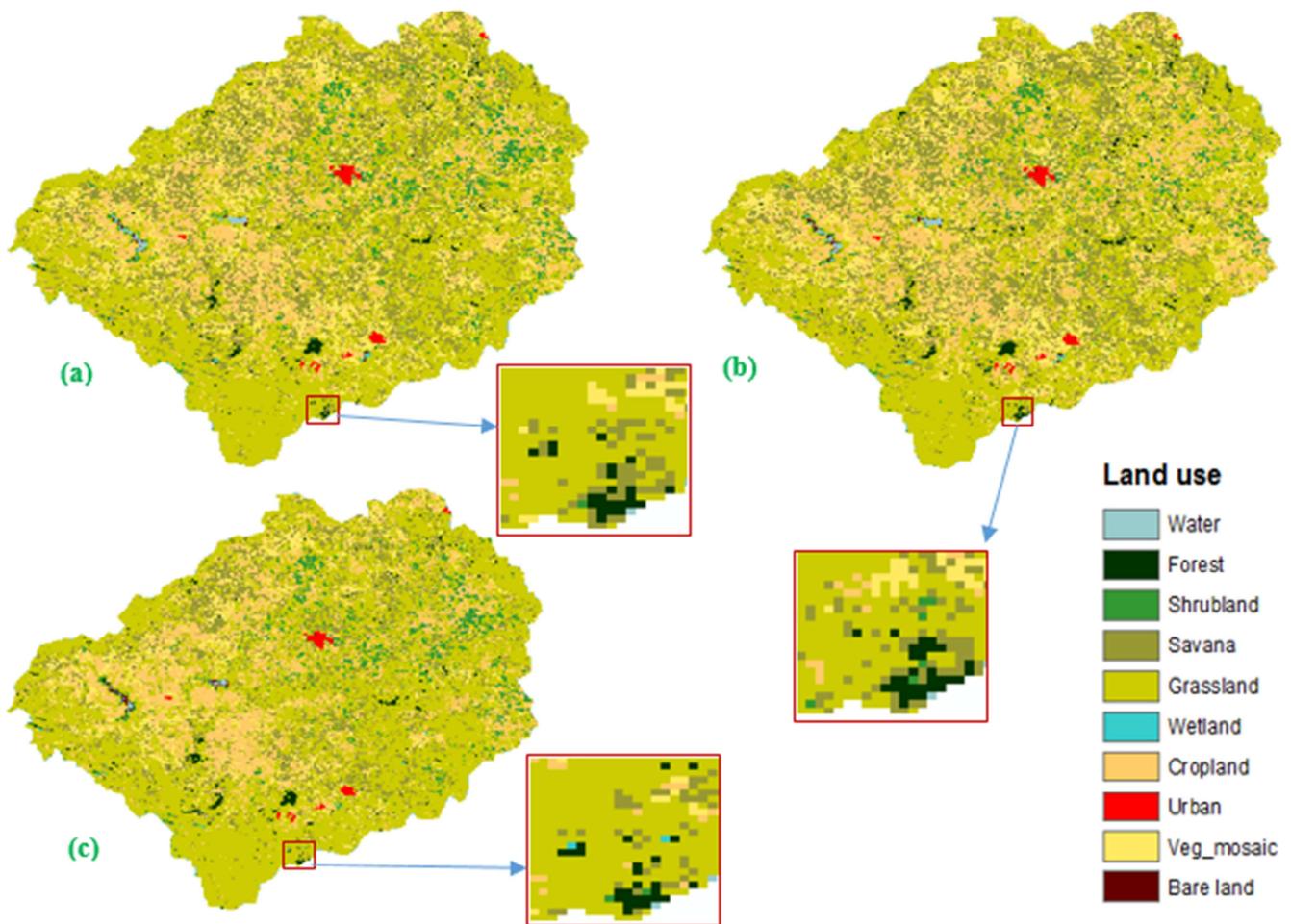
## 4.2 Land-use change

The land-use model was simulated from 2001 to 2030. Both coupled and uncoupled simulated maps for the year 2010 are evaluated against the reference land-use map for the same year. Evaluation of the coupled simulation map against the reference land-use map for 2010 showed a QD of 6.4% and an AD of 8.1%, adding up to a total disagreement of 14.5% (total agreement of 85.5%) between the two land-use maps (Table 6). Evaluation of the uncoupled simulation against the reference land-use map for the same year showed a QD of 7.5% and an AD of 8.7%, adding up to a total disagreement of 16.2% (total agreement of 83.8%), see Table 6.

Table 6. Comparison of simulated vs reference maps (GLC30) of 2010

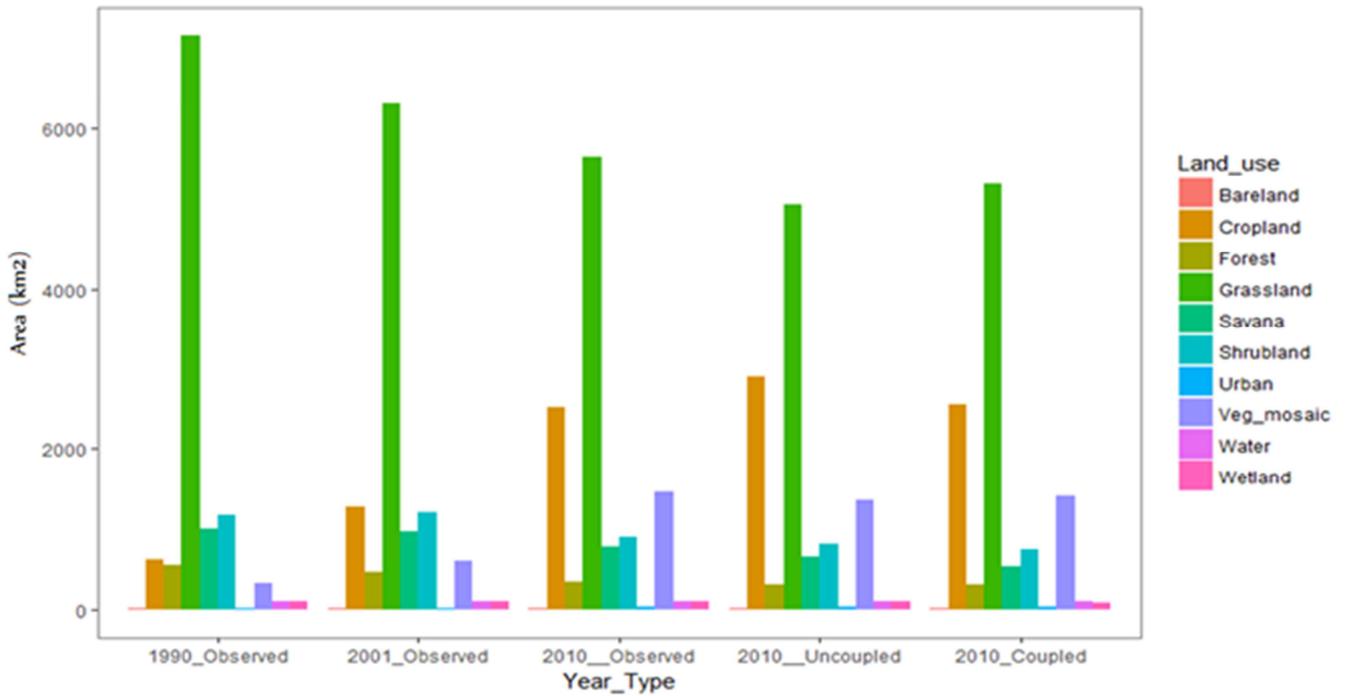
Model	Quantity and allocation disagreement			
	Components			Measure (%)
	Change simulated as 'persistence' (QD)	Persistence simulated as 'change' (QD)	Change simulated as 'change to wrong category' (AD)	Total disagreement
Coupled	2.9	3.5	8.1	14.5
Uncoupled	3.2	4.3	8.7	16.2

Results from two levels of dynamics are analyzed within the land-use model using the methodologies described thus far. In the first level, the changes in land-use, simulated using the SITE land-use change model, are observed (Fig. 8 and Fig. 9).



**Figure 8. Reference map of 2010 (a), and simulated maps of 2010 from the uncoupled (b) and the coupled (c) models.**

The second level of dynamics is the changes in grazing capacity of the grassland cover of the catchment (Fig. 9 and 10). Simulated land-use maps for the year 2010 are shown on Fig. 9 together with reference land-use maps of 1990 and 2000. As it can be seen from the figure, major land-use change trends are increases in 'Cropland' and 'Veg\_mosaic' and decreases in 'Grassland', 'Forest', 'Shrubland' and 'Savana'.



**Figure 9. Comparison of land uses from 1990, 2001, and 2010**

Quantification of trends of the grassland biomass and ecosystem services in the Thukela catchment using both the coupled and the uncoupled models is shown in Fig. 10. The figure shows that grassland biomass and the associated grazing ecosystem service in the catchment show a decreasing trend in general. The coupled model shows higher amount of biomass but lower value of grazing ecosystem service, whereas the uncoupled model shows lower amount of biomass and yet higher amount of grazing ecosystem services.

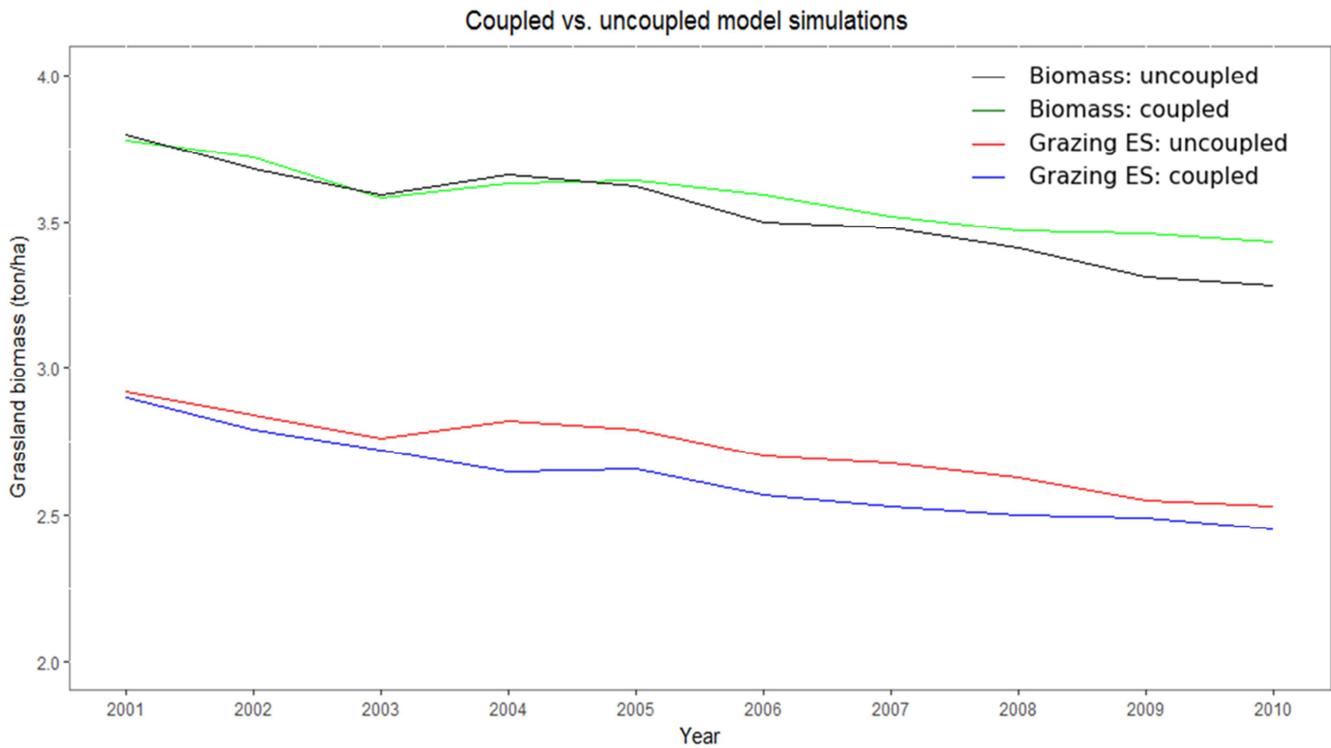


Figure 10. Trends in grassland biomass and grazing ecosystem services using the coupled and the uncoupled models

## 5 Discussion

From the perspective of hydrologic modelling, the calibration and evaluation values for the uncoupled model show NSE measures of 0.58, 0.53, and 0.52 for the calibration (1990-1994) and validation (1995-2000, 2001-2010) periods, respectively. A model performance with NSE value  $>0.5$  is often taken as satisfactory in hydrologic modelling (Moriassi et al., 2007). Accordingly, the performance of the model simulation was deemed acceptable. Likewise, PBIAS measures show values -0.17, -0.21, and -0.22 for the calibration and validation (1995-2000, 2001-2010) periods in the uncoupled hydrologic model, respectively (Table 4). Negative PBIAS values show that the simulated model generally underestimates the observed flow. However, the values are within the acceptable range (within  $\pm 25\%$ ) for advisable PBIAS measure (Moriassi et al., 2007). Evaluation of the coupled models (2001-2010) showed NSE and PBIAS performance values of 0.54 and -0.19, respectively (Table 4). Both the NSE and the PBIAS values for the coupled and the uncoupled models are relatively close, with slight improvement in favor of the coupled model in both measures.

A closer look between results of the coupled and the uncoupled hydrologic models for the period between 2001-2010 (Fig. 6) shows that the coupled model captures the observed flow, especially during high-flow seasons, better than the uncoupled

model. This is shown to be the case using results (shown in Table 5) derived from the flow hydrograph. The analysis shows that, when compared with the observed flow, the coupled model has an overall smaller percentage difference on average during high-flow seasons whereas it is relatively comparable with the uncoupled model during average and low-flow seasons (see Table 5). Better performance of the coupled model is because the dynamic changes in land-use better reflect the actual situation, as can be seen on figure 9, leading to a better simulation of the runoff generation process. The overall difference between the coupled and the uncoupled hydrologic models, as can also be seen from the performance measures in Table 4, seems marginal, however.

With regards to changes in land-use, a trend of decrease in grassland and increase in cropland can be observed from base and reference maps of 1990, 2000 and 2010 (Figs. 8 and 9). Both the coupled and the uncoupled land-use simulation results of 2010 are compared with the reference map of 2010 (GLC30). The overall performance difference, as measured using the quantity and allocation disagreements, between the coupled and the uncoupled models, 14.5% and 16.2%, respectively, is modest, and not as significant as we would expect. Results from both the coupled and uncoupled land-use change models for 2010 (Fig. 9) show notable differences in the simulation of the land-use change trend. In the uncoupled model, lower 'grassland' and higher 'cropland' allocation is shown compared to the ones in the coupled model for the same year. This is due to the fact that, in the uncoupled model, no restriction or factor is set with regards to availability of water for crop suitability. Thus, more land-use pixels (including grassland pixels) that may normally be less suitable in terms of water availability will get converted and allocated to cropland due to lack of information on water dynamics. This results in allocation of more grassland pixels to cropland in response to higher demands for the later. In the coupled version, the land-use change model gets more accurate water related constraints to compute land-use suitability for land-use allocation. Thus the coupled land-use change model constrains the suitability of pixels for cropland, for instance, on which water availability is limited. In regards to the grassland allocation, the coupled model is more optimistic on the catchment's suitability for grassland (based also on water availability input) when compared to the uncoupled model (that does not consider such an input). On the other hand, the uncoupled model allocates more land uses in response to cropland demands irrespective of water availability, i.e., due to lack of water availability information. Comparison of the coupled and the uncoupled land-use models show that hydrologic components/water availability can constrain suitability of a catchment for various land-use purposes (Fig. 9 & 10). Furthermore, the coupled versions of both the hydrologic as well as the land-use change models show modest improvement in performance when compared to their uncoupled counterparts. However, the difference between the performances could well be argued to be marginal, and thus difficult to unequivocally separate signal from noise from these results.

Unlike the marginal improvement on performances between the coupled and the uncoupled versions in the respective models, the difference in quantification of ecosystem services assessment (of grazing in this case) between results of the coupled and the uncoupled models is significant, however. The difference between the coupled and the uncoupled model

results shown, on Fig. 10, is attributed to lack of water availability information in the uncoupled model. Without feedback from the hydrologic model on the dynamics of water availability, the grassland vegetation growth could not be constrained for water demands and climatic variables. Areal coverage of a grassland from the land-use model alone would not have been enough to explicitly estimate the sustainability of the grazing ecosystem service as presented here. This is important for informed decision making on integrated management of natural resources in general and for spatially explicit quantification of catchment ecosystem services in particular.

In summary, the study shows that dynamic feedback between land-use and hydrology improves model performances only marginally. The trends both models follow were also slightly different, where the coupled model was especially better at capturing high-flows in the hydrologic model. The coupled land-use model showed slightly better performance than the uncoupled land-use model. The result of the hydrologic simulation is however not unexpected from this ten-year simulation, given that hydrologic changes are often more noticeable at large timescales of years and decades. The significant result, and the significance of the model coupling, was observed better in the simulation of dynamic feedback between the two models for assessment of the sustainability of the grazing ecosystem service potential of the grassland in the Thukela catchment. As shown earlier, availability of water together with climate variables (for suitability assessment in the land-use model) as well as yearly average biomass (for computation of the grazing ecosystem services) could not have been analyzed from either of the uncoupled models alone. Thus, besides filling the conceptual gaps in land-use and hydrologic model representations argued from the outset in this paper, model coupling provides additional potential for exploration and adds a new dimension for assessment of environmental problems (such as the ecosystem service assessment in this study) that may not be addressed from individual models alone. To the best of our knowledge, this practice is nearly non-existent, or non-reported, and only static land-use maps, from a single episode or a couple of periodical episodes, are oftentimes used to analyze land-use impacts on hydrology. Furthermore, although the magnitude of the overall land-use change impact on the hydrology seems less pronounced, a closer look at the sub-components of the flow hydrograph has shown that sub-components of the streamflow responded differently to the dynamics of the land-use (see Table 5). Likewise, hydrology is only barely, if ever, represented in land-use change models, often through the use of either precipitation or through analysis of proxies such as distance to water sources. Such practices in modelling in general, we argue, have downplayed the reported effect of the dynamics of land-use change in hydrology and vice-versa, and even more so for the assessment of ecosystem services dependent on these interacting domains.

Furthermore, to our awareness, this study is the first experiment thus far at dynamically coupling land-use change and hydrologic models. The closest modelling experiments we come across are the ones carried out by Wagner et al (2017) and Wagner et al. (2016). These studies, carried out on an Indian urban catchment, applied multiple land-use scenario maps every five or ten years for their hydrologic simulation. Although still different on conceptualization, both of these papers concluded, similar to our conclusion here, improvements in model results and model performance as a result of using

multiple (dynamic) land-uses in their hydrologic simulation. In this regard, we believe that our study establishes an opportunity for further research in the area of ecosystem services, a relatively young domain, within the framework of coupled models particularly from established domains of hydrology and land-use change.

All being said, there is ample scope for improving this study. First, besides model uncertainties, lack of high resolution and reliable data especially on socio-economic inputs will have influenced model results. Second, as is usually the case with integrated models, coupling of the two models involves several parameters, tools and techniques. The number of tools involved, the need for modifying both models at code level and a number of spatial and temporal parameters on both (such as simulation time-steps and spatial resolutions) can make model coupling technically demanding. Alternative coupling methods, for instance for pre-defined input and outputs such as OpenMI (GREGENSEN *et al.*, 2007), may be consulted in cases where less technical endeavors in data exchange, but predefined or relatively rigid, interaction between two models is desired. In spite of these limitations, however, we have noted that regardless of magnitudes, dynamic feedback of land-use change affects hydrologic response, and that dynamic feedback of hydrology affects land-use responses. Even more so, results of dynamic feedback between hydrology and land-use change affect quantification of ecosystem services in a catchment. Hence, a deserving attention should be given to the dynamic interaction of land-use and hydrology during the development of modelling concepts or modelling activities in respective models for a more accurate and explicit quantification of catchment ecosystem services.

## 6 Conclusion

The study presents an analysis of the effects of dynamic feedbacks between land-use and hydrology for the quantification of ecosystem services using an integrated modelling approach. The model integration/coupling exchanges annual aboveground biomass from the hydrologic model to the land-use model and land-use maps from the land-use to the hydrologic model. Dynamic feedback between the hydrologic and the land-use change models show marginal improvements in performance in both models (for SWIM, NSE and PBIAS values barely increased and for SITE the map-comparison statistics improved only slightly). Thus, it can be argued that coupling land-use change and hydrologic models may not be always necessary for general modelling purposes. However, the effect of dynamic feedback between hydrology and land-use change was shown more clearly to affect quantification of ecosystem services in this study. A serious modelling effort for specific needs (such as to analyze effects of land-use change on runoff generation for purposes of flooding/ peak-flow, etc.) or for quantifying catchment ecosystem services associated with land and water resources would be advised to account for the dynamic feedback between these domains. Accounting for the dynamic feedback can also serve to fill the conceptual gaps in representation of the interactions between the respective models observed in the literature. For a general practice, however, it can be argued that model integration, and thus model coupling, increases technical complexity. Thus, modelers and environmental decision makers should weigh between the need for a better performance and complexity when it comes to

practical applications of coupling. As a follow-up, we envision to add other ecosystem services into the equation and explore potential synergy and trade-off between multiple ecosystem services from the coupled models using the framework presented in this study.

### **Code availability**

All Python and R scripts developed for this study are freely available to anyone upon request through the corresponding author.

### **Acknowledgements**

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**Highlights**

- Calibrated and dynamically coupled a land-use change model and a hydrologic model
- Analyzed effects of the dynamic feedback between the two on quantification of ecosystem services
- Coupled models performed only slightly better at capturing observation on both models
- Coupled models produced a more robust quantification of catchment ecosystem services

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