Science of the Total Environment 833 (2022) 155042

Contents lists available at ScienceDirect

Science of the Total Environment

journal homepage: www.elsevier.com/locate/scitotenv

Understanding the accuracy of modelled changes in freshwater provision over time

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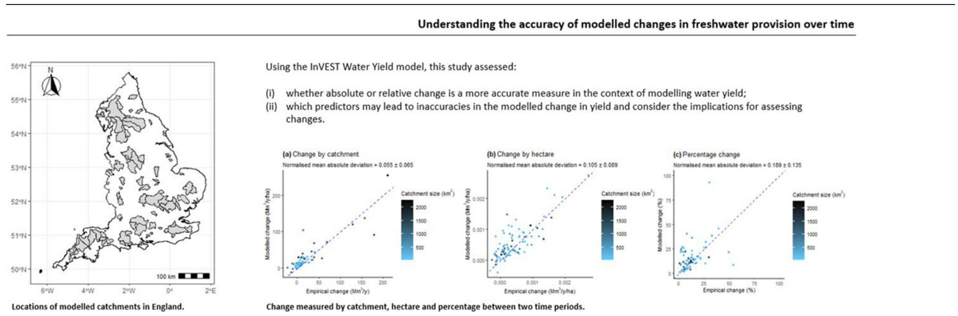
HIGHLIGHTS

- Modelled annual yields showed high accuracy, with low Mean Absolute Deviation (MAD) at the catchment and hectare scales.
- Accuracy (MAD) of modelled absolute change in water yield showed moderate fit for catchment and hectare scales.
- Anthropogenic modifications contributed significantly to the inaccuracy of change values (catchment and hectare scales).

GRAPHICAL ABSTRACT



ARTICLE INFO

Editor: Ouyang Wei

Keywords:
Water yield
InVEST
Human impacts
Model validation
Ecosystem services
Anthropogenic impact

ABSTRACT

Accurate modelling of changes in freshwater supplies is critical in an era of increasing human demand, and changes in land use and climate. However, there are concerns that current landscape-scale models do not sufficiently capture catchment-level changes, whilst large-scale comparisons of empirical and simulated water yield changes are lacking. Here we modelled annual water yield in two time periods (1: 1985–1994 and 2: 2008–2017) across 81 catchments in England and validated against empirical data. Our objectives were to i) investigate whether modelling absolute or relative change in water yield is more accurate and ii) determine which predictors have the greatest impact on model accuracy. We used the Integrated Valuation of Ecosystem Services and Tradeoffs (InVEST) Annual Water Yield model. In this study, absolute values refer to volumetric units of million cubic metres per year (Mm^3/y), either at the catchment or hectare level.

Modelled annual yields showed high accuracy as indicated by the low Mean Absolute Deviation (MAD, based on normalised data, 0 is high and 1 is low accuracy) at the catchment (1: 0.013 ± 0.019, 2: 0.012 ± 0.020) and hectare scales (1: 0.03 ± 0.030, 2: 0.030 ± 0.025). But accuracy of modelled absolute change in water yield showed a more moderate fit on both the catchment (MAD = 0.055 ± 0.065) and hectare (MAD = 0.105 ± 0.089) scales. Relative change had lower accuracy (MAD = 0.189 ± 0.135). Anthropogenic modifications to the hydrological system, including water abstraction contributed significantly to the inaccuracy of change values at the catchment and hectare scales.

Quantification of changes in freshwater provision can be more accurately articulated using absolute values rather than using relative values. Absolute values can provide clearer guidance for mitigation measures related to human consumption. Accuracy of modelled change is related to different aspects of human consumption, suggesting anthropogenic impacts are critically important to consider when modelling water yield.

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http://dx.doi.org/10.1016/j.scitotenv.2022.155042
Received 17 December 2021; Received in revised form 31 March 2022; Accepted 31 March 2022
Available online 05 April 2022

1. Introduction

Ecosystem services (ES), the benefits that people derive from nature (MEA, 2005), are fundamentally linked with the quality of peoples' lives (Pascual et al., 2017). Together with the conservation of biodiversity, safeguarding, sustaining, and improving the current provision of ES has increasingly become a focus of national and international policy (Bouwma et al., 2018; Defra, 2020a; United Nations et al., 2021). This focus has been highlighted by the formation and work of the Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services (IPBES), which aims to improve the linkages between biodiversity, ES, and policy worldwide (IPBES, 2019; Pascual et al., 2017). The European Union's (EU) Knowledge and Innovation Project also aims for an integrated system to assess natural capital and ES. Accounting in the EU seeks to fully integrate ES flows and their monetary valuation into accounting and reporting systems (La Notte et al., 2017). This requires the accurate quantification of ES, which requires clear guidelines, methodologies, standards, and long-term evidence (Guerry et al., 2015; La Notte et al., 2017; Polasky et al., 2015; Willcock et al., 2019).

Water yield (i.e., freshwater provision) in this study refers to annual water yield as annual rainfall minus annual actual evapotranspiration, with no distinction between surface and subsurface flows. Calculating and predicting the ES of freshwater provision is of vital importance, as freshwater is necessary for human consumption and crop growth, among other uses (Aylward et al., 2005; OECD, 2013; Rodell et al., 2018). Freshwater availability in a certain area is influenced by the hydrological cycle, which is driven by temperature and precipitation; the human demand for water resources for such uses as drinking, irrigation, and hydropower production; and economic factors, which affect the efficiency and amount of extraction and management (Gleick, 2018; Grizzetti et al., 2015). Freshwater supply is also intrinsically linked to other ES. For example, freshwaters provide cultural services such as recreation and tourism, and intellectual, aesthetic, and spiritual appreciation (Grizzetti et al., 2015). Regulatory services, including water purification, erosion prevention, and soil formation, are inherent aspects of functioning freshwaters (Aylward et al., 2005; Grizzetti et al., 2015). Additionally, freshwater habitats support approximately 10% of all known species, despite covering less than 1% of the Earth's surface (Strayer and Dudgeon, 2010).

Due to increasing anthropogenic pressures, such as the effects of climate change, pollution, flow regulation, and water extraction, the degradation and destruction of freshwater ecosystems are widespread and growing (Everard and Moggridge, 2012; Gleick, 2018; Strayer and Dudgeon, 2010). This results in the depletion and degradation of water resources leading to freshwater scarcity in many regions of the world. Many studies have therefore attempted to assess and model both flow and total water yield, often with the explicit aim of trying to identify areas that are likely to be vulnerable in terms of changes to water supply (e.g. Muhar et al., 2016; Rodell et al., 2018). Assessment of water supply has been undertaken qualitatively, quantitatively, or in monetary terms, and at different spatial scales (e.g. Böck et al., 2018; Muhar et al., 2016; Rodell et al., 2018). For example, Brunner et al. (2019) modelled the current and future supply of water across the whole of Switzerland.

The availability of water is important for decision and policy making at a range of scales for a range of purposes. In the UK, this has taken the form of the Government's 25 Year Environment Plan, which sets out an ambitious vision. One of its key objectives is to have 'clean and plentiful water', which focuses explicitly on water yield, having an indicator of 'achieving sustainable abstraction' (Defra, 2019a, 2019b; HM Government, 2019). For example, in England, several plans and strategies exist to ensure that there is enough water for the future needs of both people and the environment (Environment Agency, 2021). Abstraction licensing, water resources planning, and reporting require continuous assessment and modelling of the quantity of water resources, including how much abstraction the environment can sustainably supply (Defra, 2019a, 2019b) and understanding how availability may change in response to various pressures. Local assessments inform environmental status and management choices to prevent deterioration and maintain water supply. They can be used to translate higher level plans (e.g. River Basin Management Plans and the Water Abstraction Plan (Environment Agency, 2017)) into local licensing policy (Environment Agency, 2021). For example, the Catchment Abstraction Management System process assesses resource availability at specific locations to determine abstraction availability for public water supply and other sectors (e.g. agriculture) as well as contributing to strategic overview and policy decisions. Water Resources Management Plans set out how each company intends to maintain the balance between the supply and demand for water over the next 25 years at the water resource zone level, following Environment Agency guidelines (Charlton and Arnell, 2011), translating water yield from different sources (river flow, groundwater, reservoir storage) into measures of water available for supply. More recently, the National Framework (Environment Agency, 2020) identified strategic water needs for England and its regions across all sectors, using different modelling approaches. Water requirements were projected across the country by 2050 based on statistical modelling of likely supply and demand and through application of percentage changes to natural flows (to assess the amount of water available for abstraction after considering water remaining for the environment). With no action to address pressures, the national framework modelling suggests England could need up to 3435 Ml/d of water by 2050 to meet public water supply needs. Several studies have modelled anticipated changes in river flows from the catchment (e.g. Arnell and Reynard, 1996) to national scales (e.g. Kay, 2021) using different hydrological models and climate projections. Taylor et al. (2019) forecasted water yield changes in response to management and climate scenarios at the catchment scale. Such studies are used to inform and guide management and policy, to ultimately ensure the continuity of sufficient freshwater supplies.

Mapping is considered an effective way to support decision-making regarding ES, as it provides a spatially explicit representation of differences in ES provision (Böck et al., 2018), helps to decide where policy interventions may be most effective (Rieb et al., 2017), and can enable a risk-based approach of 'know', 'target', and 'manage' (OECD, 2013) at the landscape scale. In the UK, Defra (2020a, 2020b) have similarly proposed the mapping of natural capital as the best way to determine the variability in the distribution of ES provisions. Natural capital is easier to map explicitly since it is the 'stock' of current natural assets (Guerry et al., 2015), whereas ES mapping remains challenging due to the complexities of flows and beneficiaries (Rieb et al., 2017). With regard to water supply, simple inferences from land use and cover mapping are often insufficient to effectively inform policy and management regimes because the effect of land use change on water resources is extremely context specific (Zhou et al., 2015) and dependent on the exact path that water takes through the landscape as influenced by topography and soil properties. Therefore, models are often required to make assessment of likely changes and uncertainties of water supply at the landscape scale (Böck et al., 2018). Furthermore, water resource systems for supply are frequently heavily moderated, requiring a further step in the modelling chain to assess how much water is available for supply, often using outputs from hydrological models. This uncertainty is why relative change estimation is used.

However, current landscape-scale hydrological modelling often has large uncertainties and inaccuracies (Calvin and Bond-Lamberty, 2018). Therefore, the question remains how to model water yields with high accuracy across landscapes. This is especially true when modelling change of freshwater provision over time, as many processes that influence water yield change are both temporally and spatially variable (Smith et al., 2019). Precipitation, land use and land cover are critical inputs in most ES models that simulate water yield. These factors are important in determining water supply, as precipitation is the principal driver of the hydrological cycle, and the composition and configuration of land use and cover are known to have a variety of impacts on overall freshwater supply (López-Moreno et al., 2011; Maetens et al., 2012; Sun et al., 2015). The latter point has even led to the modelling of water yield based purely on land use (e.g. Hasan et al., 2020; Hassaballah et al., 2017). However, spatial differences in ES provision cannot be explained by land use alone (Han and

Dong, 2017), partly due to the complexities of hydrological processes mentioned above, but also due to model assumptions such as classifying land use types as 'pristine' or 'natural', although this is often not sufficiently nuanced (Blair and Buytaert, 2016). Other factors and predictors that may influence how land use affects water yield include climatic factors, human activities, and feedbacks between them (Calvin and Bond-Lamberty, 2018). These factors can result in large variations in model accuracy when comparing locations where these factors have differing influences. For example, in areas of the UK where snowmelt occurs, modelling hydrological variability is less accurate compared to where it does not occur (Smith et al., 2019). Due to the profound influence of human activities on freshwater supplies, including water abstraction for irrigation and water storage and management (e.g. via reservoirs), socio-hydrological models that include the dynamics of co-evolution of coupled human-water systems have risen in prominence in the last decade (Blair and Buytaert, 2016). However, very high levels of uncertainty remain in such models, and human-influenced factors rarely feature at the landscape or larger scales (Calvin and Bond-Lamberty, 2018). Therefore, it is important to gain an understanding of how accurate current models are that influence policy. To be able to improve the interpretation of models, identifying factors that cause inaccuracies is key, whether they are model-derived or extraneous. Tracking temporal and spatial changes in water yield should enable quantification of the impact of such factors, through an understanding of the important drivers of change, and the importance of the drivers in influencing model estimations.

Tracking water yield changes over time is especially important in terms of policy decisions, to try and understand how, what and where changes may occur in order to manage them. This information needs to be put simply, as it is often needs to be understood by laypeople trying to interpret model outputs. Change in water yield is frequently presented as relative (percentage) values, which are used to compare across space, time and where uncertainties create a wide range of outcomes (e.g. Lempert, 2019). They are especially useful when objectives cannot be translated into clear target indicators and values (Haasnoot et al., 2019), or where a study is focused more on non-predictive, exploratory modelling (Lempert, 2019), such as in climate change impacts studies or of alternative futures. For example, Chaplin-Kramer et al. (2019) used percentage change to plot benefit gaps for future scenarios, and Ruckelshaus et al. (2015) used percentages to relate water yield reductions to improvements in erosion control. The use of percentages is widespread, e.g. investigating the impact of climate change on water yield in 2030 and 2060 in the Lower Mekong Basin, China (Trisurat et al., 2018), as guidance for the Water for Life and Sustainability Fund in Colombia (Vogl et al., 2015) and to assess the impact of erosion from mining activities in Himachal Pradesh, India (WAVES, 2015). However, it has been argued that conservation of natural processes should rather be presented as absolute values to provide a more accurate measure of change (Baumgärtner et al., 2006; Sol, 2019). Absolute measures are useful when decision makers are focused on some invariant standard or on one or more outcomes (Lempert, 2019), such as Water Framework Directive (WFD) objectives.

Absolute and relative metrics of change are often presented together to contextualise change. Large percentage changes do not necessarily mean that this is meaningful to the system or decision of interest if the initial absolute value is low. For example, an early study of climate change impacts on the water available for supply as part of the water resources planning process found large absolute impacts of 120 Ml/d equating to a relative change of only 10%, whilst a change of 2.7 Ml/d for another water resource zone represented a huge relative impact of almost 60% (Charlton and Arnell, 2011). However, large percentage reductions in low flows may be important for determining water available to both the environment and abstraction. In the National Framework (Environment Agency, 2020), percentage changes were applied to natural flows for differing river types and at different flows. Estimated impacts and the additional capacity required to meet different pressures between regions were presented as maps of absolute values and as a proportion of the water supplied in any given water resource zone. Charlton et al. (2018) modelled how projected climate change impacts on river flow affect phosphorus concentrations, the effectiveness of planned management interventions to reduce them, and the implications for meeting WFD objectives. Both absolute values and percentage changes were mapped showing small but inconsistent increases in projected phosphorus concentrations across England. The maps of percentage change in concentrations relative to an absolute baseline identify where change in risk is greatest. Absolute changes in WFD status are necessary to assess implications for WFD objectives. Together this information informs strategic decision making at a national scale and helps to target management responses. Importantly, most phosphorus concentration estimates were found to be sufficiently high for meeting thresholds for algal growth suggesting the need for further management focused on other drivers of risk, such as water temperature (Charlton et al., 2018).

Ultimately, the choice of change metric depends on the purpose; absolute and relative changes provide different and complementary information to decision makers. Confidence in modelling results influences their utility in planning. Uncertainty and accuracy feed into this. Modelling errors will manifest in estimates of change in both absolute and relative terms. What is not understood is how accuracy emerges in the choice of representation or whether the same sources of error drive this.

The aim of this study was, therefore, to investigate how best to quantify water yield changes over time, to inform how to increase the accuracy of models at the landscape scale for future management of the water environment. Specifically, we assessed:

1. Water yield for catchments in England for two time periods.
2. Whether absolute or relative change is a more accurate measure in the context of modelling water yield. In this study absolute values refer to volumetric units of million cubic metres per year (Mm^3/y), either at the catchment or hectare level.
3. Which, if any, predictors may lead to inaccuracies in the modelled change in yield and consider the implications for assessing changes in water yield in England.

To do this, we modelled water yield in England using the Annual Water Yield (AWY) model, which is part of the Integrated Valuation of Ecosystem Services and Tradeoffs (InVEST) suite. The InVEST models are widely used physically-based models used in environmental decision-making, as they allow for comparisons of trade-offs between different ES based on changing land use/land cover scenarios. The AWY model was designed to require less parameterisation and data than some more complex hydrological models, making it easier and faster to run over larger extents with readily available datasets. As an alternative to more sophisticated models that can be resource or data intensive, AWY calculates the relative contribution of land parcels to annual water yield (Sharp et al., 2018). Additionally, the AWY model has been validated for the UK (Redhead et al., 2016) and shown that it can produce accurate estimates of water yields at a landscape scale (Sharp et al., 2018). We assessed estimation accuracy using validation data for two time periods, 1990 (1985–1994) and 2015 (2008–2017). Finally, using linear regression we assessed the contribution of predictor variables (climate, physical characteristics, and human impact) to model estimation error.

2. Methods

2.1. Study site and context

The catchments used in this study lie within England, which has undergone large changes in water consumption and abstraction since at least the 1970s (Defra, 2020a; Gorenflo et al., 2012; Walker, 2013). To investigate changes in water yield over time, we chose two time periods (for which the model was run separately) that reflect different periods of land use/cover and climate. The first time period (hereafter 'time period 1'), 1985–1994, was guided by the 1990 UK land cover map (LCM1990, Rowland et al., 2020), while the second period (time period 2), 2008–2017, was guided by the 2015 UK land cover map (LCM2015, Rowland et al., 2017). Both land cover maps (LCM) are derived from optical satellite data. The data behind LCM1990 were re-processed in 2020 using the same methods as for LCM2015, thus ensuring that change between the maps is likely to be genuine, rather than due to methodological and technological differences.

The second time period ended in 2017 as data were not available for all parameters after that year. Study regions were selected on the basis of the availability of validation data (see Validation in Section 2.2.2). If catchments were nested, one of the overlapping catchments was randomly selected to avoid bias towards smaller or larger catchments. This resulted in a total of 81 catchments across England (Fig. 1) that we used for the analyses.

2.2. Modelling water yield

2.2.1. Model setup

Annual water yield by catchment was simulated using the InVEST Annual Water Yield model (v 3.8.2). This model was designed to estimate both the amount of water and value of hydropower produced by reservoirs (Sharp et al., 2020). In brief, the AWY model uses water balances to determine yield. It uses three procedural steps in its calculation. First, it determines water balance, as the difference between precipitation and evapotranspiration, based on spatial inputs such as soil type and rainfall. Due to the difficulty of measuring actual evapotranspiration, potential evapotranspiration is used instead, which was calculated using the Budyko curve method (Budyko, 1974). Second, water yield is modified based on other forms of consumption (e.g. groundwater recharge), and is summarised at the sub-catchment level. Third, the model calculates final, combined yield at the watershed level. However, the model does not consider temporal dimensions of water supply or surface-ground interactions. For more in-depth description of the model, please see the detailed user guide (Pessacg et al., 2015; Redhead et al., 2016; Sharp et al., 2018).

The main purpose of InVEST AWY model is to enable detection of change due to modifications such as land use change (Sharp et al., 2020). It is designed to be run relatively easily with freely available data, and requires a relatively limited set of parameters. Additionally, it has been validated in the UK (Redhead et al., 2016). Altogether, this makes it a useful tool to use in this study as it can be determined as to which extra easily-accessible parameters may be required for future updates to the model, and is also a useful policy decision tool to assess changes.

Redhead et al. (2016) validated the model for a single, ten-year time period, using linear regression of modelled total water (water yield) against empirical data, and demonstrated a high level of accuracy when using

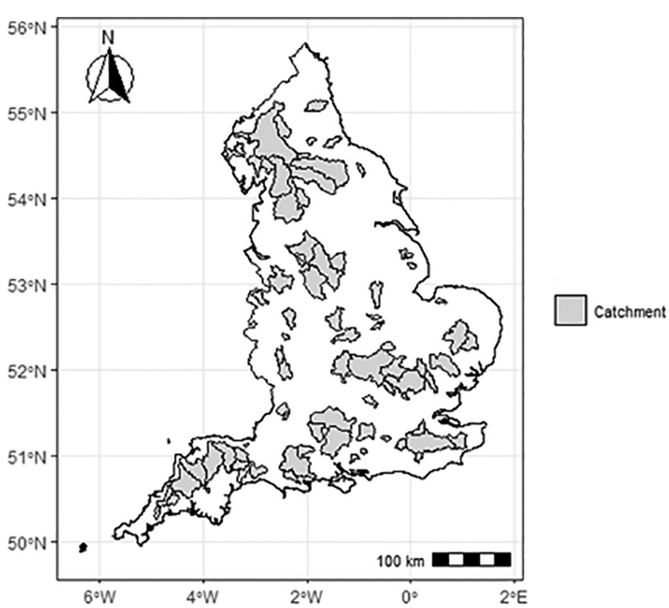

Fig. 1. Locations of the 81 catchments (grey) across England modelled in this study.

UK-scale meteorological input data. Here, we ran the model for two time periods, and assessed change between them. Table 1 shows the required inputs for the model and the specific inputs used in this study. Demand values, or water abstraction, were optional inputs for the model, which we included to improve accuracy. Water abstraction in m^3 per pixel for the LCM classes ‘arable and horticulture’, ‘urban’ and ‘suburban’ was calculated for seven regions of England (North West, North East, Midlands, Anglian, Thames, Southern and South West) using data from the Environment Agency (through Defra, 2020a, 2020b; EUROSTAT, 2020). Data were not available at regional levels for 1985, 1989 and 1990–95, therefore abstraction was calculated using percentages by region for 1995–2006 and this percentage applied to aggregated values for these years to provide estimated values. Abstraction values, or withdrawals, for public water supply, industry, mineral washing and private water supply were assigned to urban and suburban land classes following Redhead et al. (2016), and spray irrigation and agriculture were assigned to arable land, as grassland is rarely irrigated in England. We were able to provide multiple values for these land classes by splitting the input land cover codes to accommodate this complexity using Environment Agency regional boundaries that were actively used during time period 1.

2.2.2. Validation

Daily gauged flow data from the Global Runoff Data Centre (GRDC, 2020) were acquired for all stations in England that had ≥ 360 days of data for every year of the study time periods to ensure a high accuracy of the validation data. In GRDC, each station corresponds to a single catchment. The NRFA (National River Flow Archive) in the UK supply the flow data to the GRDC that is used in this study. For each station for the unnested 81 catchments, the data were summed within years, and the mean annual water yield for each catchment was calculated for each time period. These empirical results were compared to the modelled results using Mean Absolute Deviation (MAD) with normalised data. MAD was calculated by taking the mean (mathematical) absolute deviation from the 1-to-1 line resulting in values between 0 and 1; smaller values of MAD indicate higher levels of correspondence between modelled and empirical data; i.e. lower inaccuracy. MAD was used as it reflects the degree to which a model consistently reflects the validation values (Willcock et al., 2019).

2.3. Drivers of inaccuracy in modelled values

First, MAD was used to investigate overall model inaccuracies by comparing modelled values with validation data at catchment level, and hectare level (calculated using the area of the catchment) and for relative values (as percentage change) between the time periods of 1990 (1985–1995) and 2015 (2008–2017). The hectare scale estimates were examined to allow comparisons across the same scale between different catchment sizes and are simply the total water yield divided by the area of the catchment in hectares. The percentage change is the same at both the catchment and hectare scales, as the size of the catchment is constant between the two time periods.

Second, we explored possible causes of inaccuracy in the modelled changes in water yield over time. We assessed potential drivers of inaccuracy relating to human impact (including water abstraction), fine-scale land cover, physical conditions (such as area of catchment and elevation), and climate (see Table 2 for a full list of variables). Here we used the absolute volumetric values including the sign, so values could be positive or negative. We tested whether any of the predictors were correlated to the inaccuracy of the modelled change at the i) catchment and ii) hectare scales, and the iii) percentage change between the time periods using linear regression models of the residuals from the 1-to-1 line. If a predictor is strongly related to inaccuracy, this suggests that inclusion or refining the representation of that predictor, or a process involving that predictor, into the model would have resulted in improved accuracy. Several predictors used as model inputs were also included so we could examine the model's ability to effectively represent the processes involving these parameters

Table 1
Input requirements for the InVEST Annual Water Yield model, with specific inputs derived for this study. Optional inputs, including demand (abstraction), are discussed in the Model setup section.

General input data requirements			Specific inputs for this study		
Variable	Definition	Metric	Derivation of parameter	Type	Source
Precipitation	Average annual precipitation for each cell.	mm	Mean for the time period.	Spatial (raster – 1 km)	HadUK-Grid gridded climate observations for the UK (Hollis et al., 2019)
Annual evapotranspiration	Potential loss of water from the soil by both evaporation from the soil and transpiration from vegetation.	mm	Mean for each time period.	Spatial (raster – 1 km)	Climate hydrology and ecology research support system potential evapotranspiration dataset (Robinson et al., 2020)
Root restricting layer depth	Soil depth at which root penetration is strongly inhibited because of physical or chemical characteristics.	mm	Mean for each time period.	Spatial (raster – 1 km)	European Soil Database derived data (Hiederer, 2013a, 2013b)
Plant available water content	Fraction of water that can be stored in the soil profile that is available for plants' use.	Fraction between 0 and 1	Mean for each time period.	Spatial (raster – 1 km)	European Soil Database derived data (Hiederer, 2013a, 2013b)
Land use/ land cover (LULC)	Map coded with land use/land cover classes.	N/A	Two separate LULC rasters for each time period; both produced using the same methods, thus are comparable.	Spatial (raster – 1 km)	LCM1990 (Rowland et al., 2020) and LCM2015 (Rowland et al., 2017)
Catchments	Catchments of the study region.	N/A	The delineations were supplied along with flow gauge data from the GRDC.	Spatial (polygon)	GRDC (2020)
Root depth of land use/land cover classes	The depth at which 95% of a vegetation type's root biomass occurs.	mm (integer)	Pre-existing values used.	Numeric (float)	Redhead et al. (2016)
Plant evapotranspiration coefficient (*Kc*) of land use/land cover classes	Potential evapotranspiration by using plant physiological characteristics to modify the reference evapotranspiration.	Coefficient between 0 and 1.5	Pre-existing values used.	Numeric (float)	Redhead et al. (2016)
Z parameter	Seasonal distribution of precipitation.	Days	Estimated as 26.02 for time period 1 and 27.52 for time period 2. Calculated by multiplying the annual mean rainy days (precipitation amount ≥ 1 mm) for England by 0.2.	Numeric (float)	Met Office (2020)

(e.g. the model may not perform accurately where model parameters are at high or low extremes). We also included land cover and precipitation as predictor variables, to assess whether, despite being an input to the AWY model, they contributed to model inaccuracy (e.g. there may be high levels of uncertainty in the coefficients associated with certain land cover classes). Water abstraction is included in the AWY model as part of the "demand" input, and we also included it as a predictor variable (i.e. as one of the proxies of human impact). The AWY model subtracts the demand from the total modelled water yield.

Initially, univariate linear models with a single predictor were run for all residuals without intercepts (see Supplementary Materials, Tables S1–3). All variables were standardised using Z-transformations. To reduce collinearity in the full regression models, correlation between all variables was assessed using the R package *caret* (Kuhn, 2020). If variables had a Pearson's r greater than ±0.75, the variable with the lower R^2 in the univariate models was removed. Finally, full models with all remaining predictor variables were run and stepwise selection (forward and backward) using the R package *MASS* (Venables and Ripley, 2002) was used to find the most parsimonious final model. Variance Inflation Factors were investigated using the R package *car* (Fox and Weisberg, 2019); all values were <5 in the final models, indicating a low level of collinearity. The intercept was included in the final models, as it is assumed that were factors outside of our analysis impacting the overall predictive ability of our models. Spatial analysis was conducted in either R v.4.0.3 (R Core Team, 2020) or QGIS v3.4 (QGIS Development Team, 2021). All statistical analyses and data visualisations were conducted in R (R Core Team, 2020).

3. Results

The modelled mean annual water yield for both periods showed a low MAD (low accuracy) when compared against validation data (Fig. 2). Normalised MAD was 0.013 (±0.019) and 0.012 (±0.020) at the catchment level for periods 1 and 2 respectively. At the hectare scale, MAD was 0.036 (±0.030) and 0.030 (±0.025) for periods 1 and 2, respectively. For change between the time periods (see Fig. 3) the most accurate model was the absolute change at catchment scale (MAD = 0.055 ± 0.065), followed by absolute change at hectare scale (MAD = 0.105 ± 0.089), although the MAD for percentage change was much higher (MAD = 0.189 ± 0.135). Further details of the spatial difference between modelled and empirical values are mapped in Supplementary Materials, Figs. S1 and S2.

Linear regressions to identify predictors of water yield change inaccuracy (Table 1 and Fig. 4) showed that the best-fitting model was at the catchment scale was moderate (R^2 = 0.41), followed by the hectare scale (R^2 = 0.40). The model with the least variation accounted for was percentage change, with a weaker model (R^2 = 0.28). Results identified both positive and negative relationships, indicating a source of overestimation or underestimation of change, respectively. At the catchment scale, three predictors were significant at $p < 0.05$: the amount of water abstraction in time period 1 and the number of reservoirs per catchment had positive effects (i.e. overestimation of change in catchments with more abstraction and reservoirs), while 'all water barriers' (sum total of culverts, dams, fords, ramp bed sills, sluices, weirs, and others) had negative effects (underestimation inaccuracy). Sluices, fords and 'other water barriers' were positively significant at the $p < 0.10$ level. At the hectare scale, eight predictors were significant at the $p < 0.05$ level; five were positive: arable land percentage, water withdrawal in time period 1, number of reservoirs, improved grassland percentage and other water barriers (e.g. hydroelectric deviations, mobile gates, concrete, screen). The three predictors showing negative relationships were: 'all water barriers', mean air temperature, and catchment area (ha). Longitude and barrier-free length share (stream fragmentation) were significant and negative, and woodland significant at the $p < 0.10$ level and positive. At the relative (percentage) scale, only impervious built-up and improved grassland were found to be positively and negatively significant at the $p < 0.05$ level related to residuals from the 1:1 line, respectively. Flow ratio was significant and positive, and precipitation was significant at the $p > 0.10$ level and negative (Table 3).

Table 2
Predictor variables used to investigate the inaccuracy of the modelled values in the InVEST Annual Water Yield models. Variables were calculated as mean values for each catchment.

Type	Variable	Further description	Type	Pre-processing	Source
Human impact	Water abstraction	Total abstraction (million m^3).	Numeric (float)	Total water abstraction between 2008 and 2017. See Section 2.2.1 for details.	Environment Agency through Defra (2020a, 2020b) and EUROSTAT (2020)
	Stream fragmentation	Artificial barriers (weirs and dams only) that disrupt flow of waterways as barrier free length and barrier free length share. The latter refers to the proportion of the total river network length.	Spatial (polyline)	Mean barrier free length and share calculated per catchment.	Jones et al. (2019)
	Freshwater barriers	Individual locations of barriers by type (culverts, dams, fords, ramp bed sills, sluices, weirs, and others).	Spatial (point)	The number of barriers by type, and collectively, summed per catchment.	AMBER European Barrier Atlas (AMBER Consortium, 2020)
	Reservoirs	Number of reservoirs.	Numeric (integer)	Summed per catchment.	Global Reservoir and Dam (GRanD) v1.3 Database (globaldamwatch.org, Lehner et al., 2011)
		Maximum storage capacity of all reservoirs (km^3).	Numeric (float)		
	Flow ratio	Flow ratio between wet (October to December) and dry season (January to September).	Numeric (float)	Calculated as the mean between October 1994 to September 2017.	GRDC (2020)
Land cover and physical	Impervious density	Percentage of sealed area (2018).	Spatial (raster – 10 m)	Land cover was calculated as a percentage of the total catchment. Classes aggregated were based on Redhead et al. (2016).	Copernicus High Resolution Layers (Langanke et al., 2018)
	Impervious built-up area	Binary product of where sealed areas have built-up areas (2018).			
	Arable		Spatial (raster - 25 m)		Land Cover Map 2015 (Rowland et al., 2017)
	Improved grassland				
	Semi-natural	Other grasslands (rough, calcareous, acid and heather), fen, marsh and swamp, heather and bog land covers aggregated.			
	Woodland	Coniferous and broadleaved woodland aggregated.			
	Urban and suburban				
	Area	Area (km^2)	Spatial (polygon)	Calculated as total area by catchment.	GRDC (2020)
	Elevation	Elevation (m)	Spatial (raster - 50 m)	Calculated as mean elevation by catchment.	Ordnance Survey 50 m Digital Terrain Model (Ordnance Survey, 2019)
Climate	Air temperature	Average daily mean temperature annually (°C). Average daily minimum temperature annually (°C). Average daily maximum temperature annually (°C).	Spatial (raster - 1 km)	Mean calculated 1985 and 2018.	HadUK-Grid gridded climate observations (Hollis et al., 2019)
	Precipitation	Total precipitation annually (mm).			
	Sunshine duration	Duration of bright sunshine annually (hours).			
	Wind speed at 10 m	Average hourly mean wind speed a 10 m above ground level annually (knots).			
	Sea level pressure (mean)	Average hourly mean sea level pressure annually (hPa).			
	Relative humidity (mean)	Average hourly vapour pressure annually (%).			
	Vapour pressure (mean)	Average hourly mean vapour pressure annually (hPa).			
	Days of ground frost	Number of days when the grass minimum temperature is below 0 °C.			
	Days of snow lying	Number of days with >50% ground covered by snow.			

4. Discussion

Two distinct findings emerged from the results of our study. First, modelling of changes in freshwater provision was most accurate when represented as absolute values, rather than percentage (i.e., relative) values. This can result from the sensitivity of percentage change to low initial values, potentially exaggerating inaccuracies for percentage change, compared to those for absolute change. The implications could reach beyond the study area of this study, with the results indicating that caution should be exercised when using percentage change metrics alone, and we strongly recommend that absolute values should also be assessed. As absolute values can be a more accurate representation of change than relative values, the implications of reporting at the best accuracy at larger scales/remits, e.g. internationally, are important. Thus, absolute values can provide the most robust evidence that is used to guide national or transnational policy and initiatives. Presenting absolute values of change in assessments can guide management measures more accurately and be used to assess against policy-relevant standards. This is especially true when the accuracy of the change is of vital importance, such as in the case of expected shortages in agricultural irrigation or drinking water, or at times when minimum values are important, such as seasonal low flow. Considering freshwater supply in terms of absolute scarcity allows quantification that can be related to human consumptive needs and is necessary for calculating mitigation measures in changing watersheds. There is utility in presenting percentage values, as these can make the comparisons between temporally or geographically different locations easier to interpret and can also be more understandable for policy makers, especially when the resulting decisions relate environmental concepts to economics (Baumgärtner et al., 2006). Our results suggest that ease of interpretation comes at a cost in terms of model accuracy. However, for policy and decision-making, it is important to understand whether the level of difference in accuracy between relative and absolute values will affect the outcome of an investigation and on any decisions made. The authors suggest that confidence in any estimates is paramount, and this can be communicated through the use of both types of values, whilst improving the understanding of what drives differences. Stakeholder confidence can be increased through the improvement of estimation error.

Our second major finding is that variables related to human consumption of water, or human-driven landscape change, have the greatest impact on the residuals when investigating the accuracy of predicting changes in water supply. These regression models investigated the predictors of inaccuracy in modelled annual water yield change using the residuals as the independent variable in a series of linear regression using catchment, hectare, and percentage values using a variety of relevant predictors. These models ranged from a moderate R^2 of 0.41 and R^2 0.40 for the catchment and hectare level models, to a weaker R^2 of 0.28 for the percentage level model. The

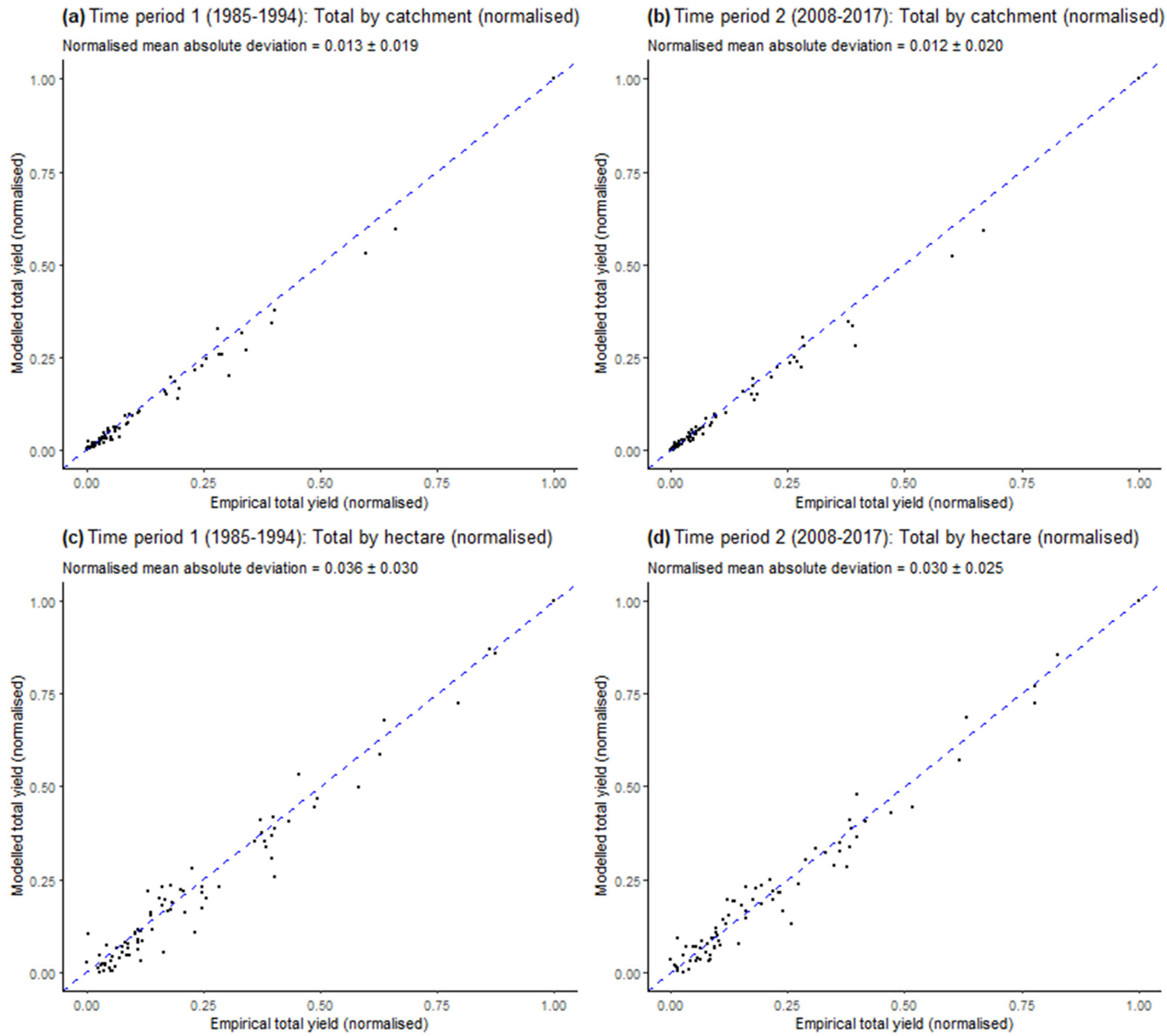

Fig. 2. InVEST modelled total annual water yield (millions of cubic metres per year (Mm^3/y)) against empirical gauged water yield for 81 catchments for (a and c) time period 1: 1990 (1985–1995) and (b and d) time period 2: 2015 (2008–2017) and by total yield per catchment (a and b) and per ha (c and d). The normalised mean absolute deviation is shown under each graph's title. The 1–1 line is shown as a blue dashed line. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

results suggest that deviations in modelled annual catchment water yield from validation data can be explained in part by human modification in hydrological processes, making anthropologically influenced processes critically important factors to consider in water yield modelling and data collection, as hypothesised by Redhead et al. (2016). Water abstraction activities and major artificial modifications (e.g. water barriers and number of reservoirs) were also particularly significant factors. Smith et al. (2019) reached similar conclusions when modelling streamflow in the UK and found that excluding artificially modified processes from the models resulted in unrealistic flow patterns. To account for the effects of human impacts, Pokhrel et al. (2015) used a model that combined human impacts, groundwater pumping, and surface interaction and runoff to model water yield. They found that adding human impacts increased the accuracy of the model and the results matched the observed data much better. However, as noted by Pokhrel et al. (2015), the coarse resolution (~100 km^2) of their model is a limitation, which means that such a model would not be sufficiently accurate at the catchment or hectare level, and so interpretation of the model at the landscape-scale would be uncertain.

The reasons for inaccuracies at the catchment level have previously been highlighted by studies that have focused on individual catchments to assess local level human impacts. For example, Xin et al. (2019), who focused on the Huifa River basin in China, identified how reservoirs affect streamflow. The authors found that the presence of reservoirs, among other human factors, had a dramatic effect on intra-annual variability, causing streamflow to decrease in every season. This was most notable during the irrigation season (May to July), when large amounts of water stored in the reservoirs were used for agriculture. Similar findings were also found in the Vu Gia Thu Bon River basin in Vietnam, and across the UK, by Firoz et al. (2018) and Tijdeman et al. (2018), respectively. In both cases, the intensity and frequency of droughts downstream depended strongly on the hydropower operations of reservoirs and abstractions. One of the challenges is that management interventions tend to be local, not catchment wide. For the River Deben in England, Hutchins et al. (2021) demonstrated a clear improvement in water quality simulations when specific local knowledge of hydrology and flow routing was included. This offers greater insights and confidence for management decisions, but the greater information requirements can be prohibitive at much larger scales. Frameworks that use large-scale screening studies and then increasingly refined modelling, proportional to local problems, allow more appropriate management solutions to be developed (Hutchins et al., 2021) and

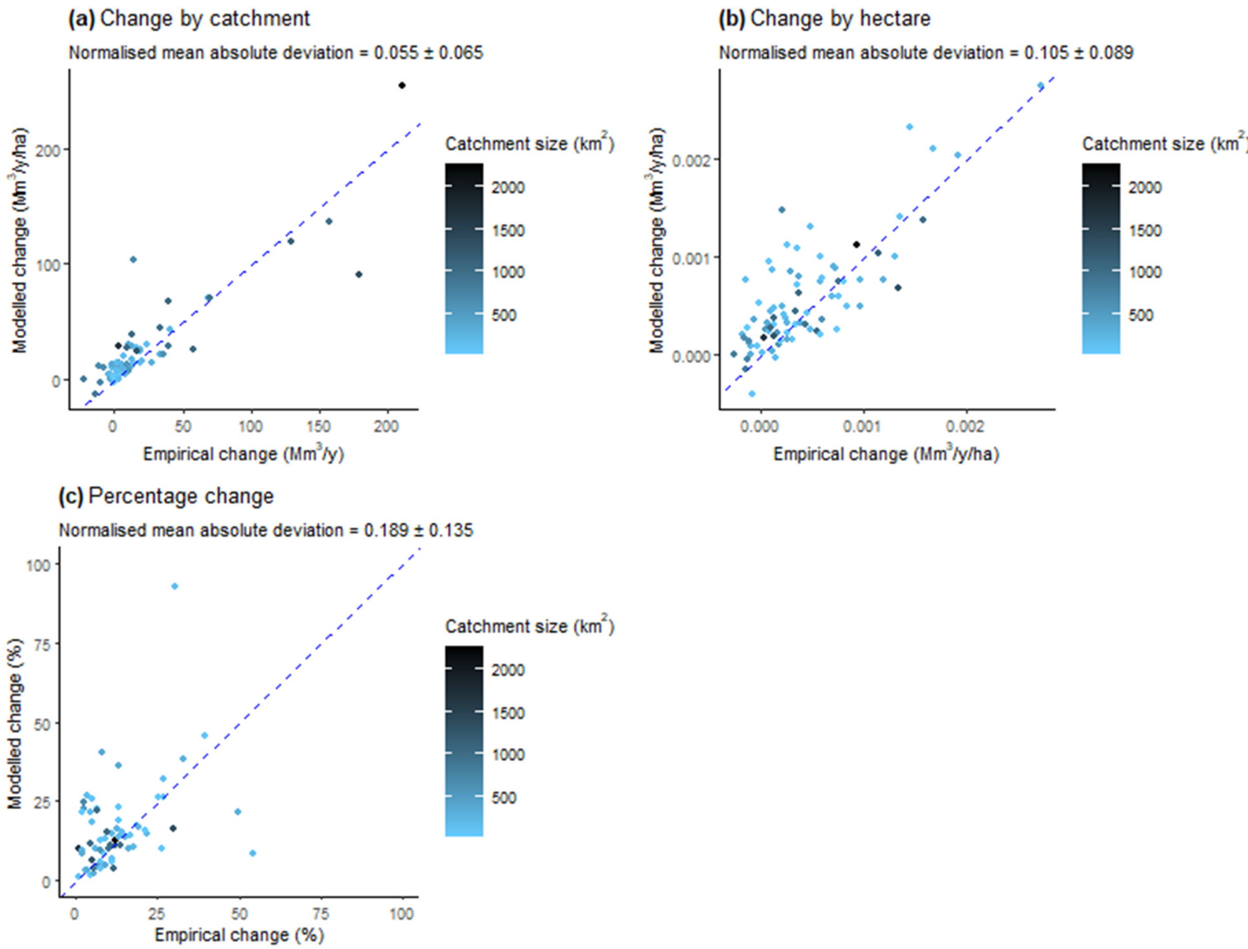

Fig. 3. Plots showing change of modelled annual water yield against empirically observed changes in yield between two time periods: 1990 (1985–1995) and 2015 (2008–2017). Graphs show this change as (a) water yield at the catchment scale, (b) water yield at the hectare scale, and (c) percentage change. The size of each catchment is marked from the smallest as light blue to largest as dark blue. The normalised mean absolute deviation is shown below the title of each graph. No normalisation was carried out prior to comparing the change between the two periods. The 1–1 line is shown as a blue dashed line. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

would allow the inaccuracy at the catchment level to be examined in greater depth.

Our study also found that, in contrast to woodland cover, which was not a significant predictor of the residuals, percentage cover of agricultural land (in the form of cropland and improved grassland) had a significant positive effect on the deviation from the validation data, indicating a positive relationship between agricultural land and residuals. This suggests that the more agricultural land there is in the catchment, the more likely the model is to predict that change was more positive than was observed, which is in agreement with Redhead et al. (2016). This overestimation due to agricultural land cover is likely due to the differing conditions and managements of agrarian land, properties of which differ greatly, showing high variability depending on factors such as stocking densities, crop types and rotations, and management activities such as tillage (O'Connell et al., 2007). The model is parameterised at the landscape scale, with a single parameter for 'average' cropland and improved grassland. However, the aforementioned runoff-affecting farm managements are decided at a local (i.e. farm-level) scale by individual actors (Blair and Buytaert, 2016), meaning this variation cannot be mapped adequately at the landscape scale without sufficient knowledge. This variation among different farms could be the reason for increased deviation (i.e. overestimation) when comparing modelled data with validation data. This could be improved by separating agricultural land into different crops and deriving parameter values for each type, whilst being mindful of management (e.g. crop rotation) for differing years. These issues may explain why the area of agricultural land was found to be a significant predictor of inaccuracy as it is a more modified land cover type, as opposed to the other less-intensive land covers that were included as predictors. Ultimately, the intensive use of agricultural land makes feedback with water processes much more dynamic and variable (Calvin and Bond-Lamberty, 2018), and their modelling at the landscape scale challenging. However, these aspects are beginning to be explicitly considered in landscape socio-hydrological landscape models (Blair and Buytaert, 2016; Wada et al., 2017).

Our results suggest that the relatively simple set of parameters used by the AWY model are a good basis for modelling changes in annual water yield generally, indicating the usefulness of the InVEST AWY model. However, they also show that the model could likely be improved by further considering human influence factors at the landscape scale, wherever in the world the model is being used. The AWY model already includes abstraction, which was a significant predictor of inaccuracy in the change between modelled water yields. Therefore, this suggests that uncertainty in the value is not an issue, but that it is not represented accurately in the model. That is, if we have the amount abstracted in the model but this amount is related to inaccuracy, uncertainty in that value will not lead to a significant effect on inaccuracy. Additionally, water abstraction data can be difficult to obtain (e.g. Larsen et al., 2019), assuming it has been collected at all. Internationally, data quality may thus be limiting when validating for previous time periods. Specifically, we found that water abstraction and number of reservoirs showed significant positive relationships with model inaccuracy for absolute temporal change, at both hectare

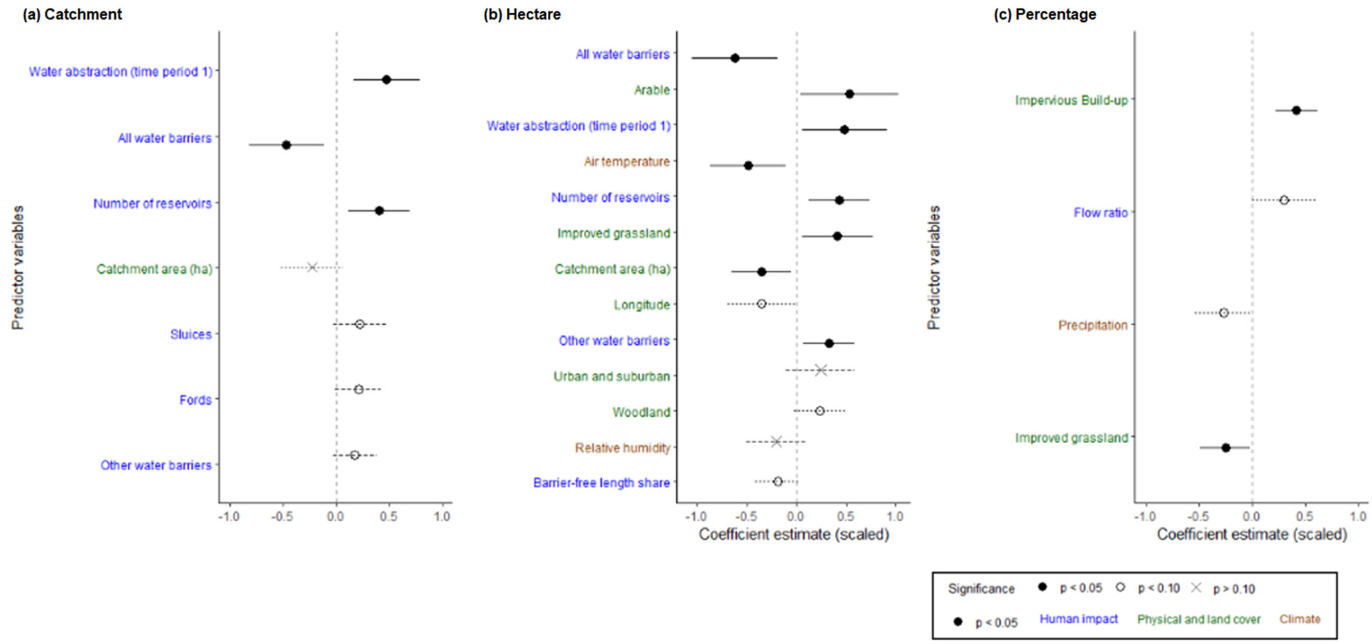

Fig. 4. Dot and whisker plots showing significance of the predictors of inaccuracy in modelled annual water yield change using linear regression with standardised variables, with stepwise selection of the most important variables. Scaled model coefficients are shown with CI whiskers for Table 1, ordered by magnitude of absolute estimate size for change by (a) catchment, (b) hectare, and (c) percentage (intercepts not shown). A positive value represents a source of overestimation and a negative a source of underestimation. Colours of variable names on the y-axis represent types of predictor: blue for direct human influence-related, green for physical and land cover related, and brown for climate related. Whereas urban and suburban and impervious built-up areas are grouped here under land cover, it must be noted that they are also indicators of human impact. Significance is denoted by shape: solid circle representing $p < 0.05$, hollow circles representing $p < 0.10$ and crosses representing $p > 0.10$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 3
Predictors of inaccuracy in modelled annual water yield change, identified using linear regression with standardised variables, with stepwise selection of the most important variables. Estimates and Confidence Intervals (CI) are shown. Predictor variable rows in bold indicate where the significance was $p \leq 0.05$. See Fig. 4 for dot and whisker visualisation.

Predictors	Residuals from change by catchment			Residuals from change by hectare			Residuals from percentage change		
	Estimates	*CI*	*p*	*Estimates*	*CI*	*p*	*Estimates*	*CI*	*p*
(Intercept)	0.00	−0.18–0.18	1.000	−0.00	−0.19–0.19	1.000	−0.00	−0.19–0.19	1.000
Water abstraction (Era 1)	**0.47**	0.16–0.79	0.004	0.49	0.05–0.92	0.029			
All water barriers	**−0.46**	**−0.82 to −0.10**	**0.012**	**−0.62**	**−1.06 to −0.18**	**0.006**			
Number of reservoirs	**0.41**	**0.12–0.70**	**0.007**	**0.43**	**0.12–0.75**	**0.008**			
Catchment area (ha)	−0.23	−0.53–0.08	0.14	**−0.35**	**−0.66 to −0.05**	**0.024**			
Sluices	0.22	−0.03–0.47	0.085						
Fords	0.21	−0.01–0.43	0.058						
Other water barriers	0.18	−0.03–0.39	0.09	**0.33**	**0.07–0.59**	**0.014**			
Arable				**0.54**	**0.03–1.04**	**0.037**			
Air temperature				**−0.49**	**−0.87 to −0.10**	**0.014**			
Improved grassland				**0.42**	**0.06–0.78**	**0.024**	**−0.25**	**−0.49 to −0.02**	**0.036**
Longitude				−0.35	−0.70–0.00	0.053			
Urban and suburban				0.24	−0.11–0.60	0.17			
Woodland				0.23	−0.03–0.50	0.081			
Relative humidity				−0.2	−0.52–0.11	0.198			
Barrier-free length share				−0.19	−0.42–0.04	0.098			
Impervious Build-up							**0.42**	**0.22–0.62**	**<0.001**
Flow ratio							0.3	−0.00–0.61	0.053
Precipitation							−0.27	−0.54–0.01	0.057
R^2 / R^2 adjusted	0.411 / 0.354			0.404 / 0.288			0.280 / 0.242		

and catchment scales, while water barriers were a negative predictor in both cases. The number of reservoirs and water barriers are not included as inputs in the AWY model, and their inclusion could improve model accuracy. Within European countries, especially those in the EU, some of these datasets (e.g. water barriers) are openly available, which means that their inclusion as additional parameters in the model would be possible. This is unlikely to be the case, however, for all countries internationally, across all datasets, therefore implications on accuracy on models depending on context need to be considered.

While our results point to factors that could be included in models to reduce their inaccuracy in terms of deviance, the R^2 values of the predictive linear regression models identifying drivers of residuals in the relationship between modelled and measured changes suggest that more variation could be explained by other factors that remain to be explored. These factors may be current limitations to the accuracy of the findings. We strongly suspect such factors are likely human or geologically induced, as these are factors are specifically noted in InVEST user's guide with an indication that may not be well captured. Current model parameters could be supplemented with further, related variables, as these could be a source of variation in such processes as in subsurface drainage, thus adding more limitations to the accuracy of the findings presented here. For example, in karst landscapes – those created from the dissolution of carbonate rocks, from which phenomena such as caves and sinkholes can form (Ford and Williams, 2013) - water supply protection is a major challenge, due to being highly vulnerable to environmental and human changes (Farrant and Cooper, 2008; Lv et al., 2020). Karst rock types are widespread across the UK (see Fig. 1 in Farrant and Cooper, 2008), therefore any changes in the condition of these areas could dramatically change water supply in certain locations, data of which was not included in this study. For other potential sources of error, including spatial and temporal, please see Supplementary Materials, Section 3.

Dynamic feedbacks between human activities and water systems may also not have been considered, which is often an issue in socio-hydrological modelling studies at larger scales (Hassaballah et al., 2017; Sivapalan et al., 2014), possibly overlooking locally important decisions made by individual actors in individual catchments (Blair and Buytaert, 2016). Additionally, inaccuracies may have been present in the validation data, as water can bypass gauging stations in various ways, e.g. pipelines and floods. In terms of consumptive abstraction, the model will correctly predict that the water was there, but it does not appear in the validation data because it has been taken out of the system, causing an apparent overestimate. This issue with validation data, and our results of human impact having effects on model deviance, suggest that the most populated catchments would have the some of the least accurate modelling, though these are areas where accurate models are most important across the world.

Building on the results of this work, there are several potential avenues for future research. As the temporal difference between the modelled time periods was probably not long enough to draw conclusions about long-term climatic changes, future studies could increase the number of years between the time periods. However, this may be difficult due to the necessity of empirical data required for accurate modelling, for example water abstraction rates, and the need for consistent land cover maps for each time period. It would also be useful to extend the study to larger regions, both in terms of number of catchments and geographical extent, as this study only covered England. Such future research could include modelling in different biomes, or investigating different types of catchments, e.g. by land cover heterogeneity, areas of extreme climatic variability or those not constrained by gauge data. We did not explore the link to the condition of the catchment in this study, but such metrics could be included in the future e.g. by making plant available water capacity dynamic.

5. Conclusion

Due to the increasing pressures on freshwater demand and supply from population growth and climate change, there is a need for future management plans to be more adaptive and flexible (Everard and Moggridge, 2012; Gleick, 2018). Our study suggests that modelled absolute values need to be presented alongside percentage values when quantifying change in freshwater provision. The use of each will depend on the context and purpose of the particular management decision. Accuracy of change estimates depends on different drivers and highlights their complementarity for understanding potential management choices. There is a need to incorporate more of the influence of human activities and consumptive use into landscape-scale water yield models. As demonstrated here, the InVEST AWY model provides a robust basis for modelling annual water yield, although incorporating a better understanding of anthropological impacts could lead to improved reliability in predicting changes in water yield.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This work was supported by BESTMAP under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 817501). The views expressed in this paper are those of the authors and do not necessarily represent the views of the Environment Agency or other institutions. The authors are thankful to the anonymous reviewers for their helpful comments.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2022.155042.

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