

National scale evaluation of the InVEST nutrient retention model in the United Kingdom

Article

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19 Abstract

- 20 A wide variety of tools aim to support decision making by modelling, mapping and quantifying
- 21 ecosystem services. If decisions are to be properly informed, the accuracy and potential limitations
- 22 of these tools must be well understood. However, dedicated studies evaluating ecosystem service
- 23 models against empirical data are rare, especially over large areas. In this paper, we report on the
- 24 national-scale assessment of a new ecosystem service model for nutrient delivery and retention, the
- 25 InVEST Nutrient Delivery Ratio model. For 36 river catchments across the UK, we modelled total
- 26 catchment export of phosphorus (P) and/or nitrogen (N) and compared model outputs to
- 27 measurements derived from empirical water chemistry data.
- 28 The model performed well in terms of relative magnitude of nutrient export among catchments
- 29 (best Spearman's rank correlation for N and P, respectively: 0.81 and 0.88). However, there was
- 30 wide variation among catchments in the accuracy of the model, and absolute values of nutrient
- 31 exports frequently showed high percentage differences between modelled and empirically-derived
- 32 exports (best median absolute percentage difference for N and P, respectively: ± 64%, ± 44%). The
- 33 model also showed a high degree of sensitivity to nutrient loads and hydrologic routing input
- 34 parameters and these sensitivities varied among catchments.
- 35 These results suggest that the InVEST model can provide valuable information on nutrient fluxes to
- decision makers, especially in terms of relative differences among catchments. However, caution is
 needed if using the absolute modelled values for decision-making. Our study also suggests particular
- 38 attention should be paid to researching input nutrient loadings and retentions, and the selection of
- 39 appropriate input data resolutions and threshold flow accumulation values. Our results also
- 40 highlight how availability of empirical data can improve model calibration and performance
- 41 assessment and reinforce the need to include such data in ecosystem service modelling studies.

42 Keywords

- 43 Ecosystem services, nutrient delivery, runoff, eutrophication, river, land cover
- 44

45 Abbreviations

- 46 BRE Beale ratio estimator, CEH-GEAR centre for ecology and hydrology gridded estimates of areal rainfall,
- 47 DEM digital elevation model, IHDTM integrated hydrological digital terrain model, InVEST integrated
- 48 valuation of ecosystem services and tradeoffs, LCM2007 land cover map 2007, LULC Land use/land cover,
- 49 NDR nutrient delivery ratio, NRFA national river flow archive, TFA threshold flow accumulation, UKCP09 -
- 50 UK climate projections, WIMS water information management system, WWTW wastewater treatment
- 51 works

52 **1.** Introduction

53 The ecosystem services concept is increasingly widely applied by decision makers seeking to assess 54 the likely impacts of environmental change on human health and wellbeing (Braat and de Groot 55 2012; Tallis et al. 2008). For ecosystem services to be useful in practice, they must be quantified and 56 mapped to identify the risks, impacts and potential trade-offs associated with predicted or known 57 environmental change, or among different change scenarios (Malinga et al. 2015). To achieve such 58 assessments, a wide variety of methods and tools have been developed to map, quantify and value 59 the provision of ecosystem services (Fisher et al. 2009; Malinga et al. 2015; Seppelt et al. 2011; 60 Sharps et al. 2017).

61 In recent years, many ecosystem service modelling tools have become freely available to the global 62 user community. This overcomes issues surrounding proprietary software and data formats, and 63 enables model development and application to benefit from increased data and model sharing, 64 cloud computing facilities and a larger user community (Feng et al. 2011). Critically, these tools 65 model multiple services, allowing users to take a multi-criterion approach to decision-making (Keller 66 et al. 2015). Whilst the free and open-source nature of such tools brings many advantages, it allows 67 users to run a wide range of models, and obtain results, with little knowledge of the modelling 68 process or expertise in the subject area. A potential pitfall is that users may not familiarise 69 themselves with the intended use and limitations of the model before using it, and may be unaware 70 of the uncertainty associated with results that they incorporate into decision making processes 71 (Willcock et al. 2016). Whilst a body of literature has begun to emerge exploring the strengths and 72 weaknesses of these models (Dennedy-Frank et al. 2016; Redhead et al. 2016; Sharps et al. 2017; 73 Willcock et al. 2016) the number of studies seeking to validate and explore the sensitivities of 74 ecosystem service models remains limited (Hamel et al. 2017; Maes et al. 2012; Malinga et al. 2015; 75 Schulp et al. 2014; Seppelt et al. 2011), especially over the large (i.e. regional to national) spatial 76 scales at which much resource management policy is formulated (e.g. Wilby et al. 2006). Such 77 studies are vital in providing user communities with the information required to choose the tools 78 that are most appropriate for their particular situation, to use them correctly, and to understand 79 associated uncertainties (Willcock et al. 2016). They can also provide valuable information on 80 potential data sources for parameterising models, and help to focus data acquisition by revealing 81 which parameters have the most influence on model accuracy. As a result, recent reviews have 82 identified that one of the key obstacles to successful ecosystem service mapping and 83 implementation into decision making processes is the comparative scarcity of validation or 84 measurements of uncertainty in many applications of ecosystem service models (Maes et al. 2012; 85 Malinga et al. 2015; Schulp et al. 2014; Seppelt et al. 2011)

87 Freshwater ecosystem service models that assess how land management affects water quantity and quality have the advantage of using physical variables that are commonly used in hydrologic 88 89 modelling, even though these contribute to a wide range of different final services, from recreation 90 to human health (Keeler et al. 2012). One of the most frequently modelled services is nutrient 91 retention, which represents the reduction in nutrient loads between sources and receiving 92 watercourses, due to biogeochemical processes involved in nutrient transport. Models of nutrient 93 retention (e.g InVEST, ARIES, LUCI (Sharps et al. 2017; Vigerstol and Aukema 2011)), typically use a 94 hydrologic module representing nutrient retention processes or, where available, direct outputs 95 from more complex nutrient models (e.g. SWAT, RHESSys, see reviews in Breuer et al. (2008); and 96 Shepherd et al. (1999)). When the modelling approach includes quantitative estimates of nutrient 97 transport and retention, it becomes comparatively easier to validate models, because 98 measurements of water chemistry are, in many countries, collected by environmental bodies and 99 the water industry and these can be used to estimate watercourse loads for comparison with model 100 outputs. Whilst this approach falls short of measuring a final ecosystem service (Keeler et al. 2012), 101 it is an important step in providing the biophysical underpinning for any further assessments of 102 ecosystem service value.

103 In this study, we used data from UK national monitoring to perform a thorough evaluation of the 104 recently released nutrient retention tool of the Integrated Valuation of Ecosystem Services and 105 Tradeoffs (InVEST, Sharp et al. 2016) ecosystem service modelling suite. InVEST is widely used for 106 modelling multiple ecosystem services and considering trade-offs (e.g. Bai et al. 2013; Leh et al. 107 2013; Nelson et al. 2009; Sánchez-Canales et al. 2012; Sharps et al. 2017) and is free and open-108 source. We used national scale, spatially distributed data (of the sort available to most potential 109 users) for model inputs and performed validation against a long-term, empirically-measured dataset. 110 Our objectives were 1) to examine the sensitivity of the model to variation in input parameter 111 values, spatial resolution and data sources, and 2) to determine the accuracy of the model against 112 empirical data when using the most informative combination of input parameter values, for both 113 phosphorus (P) and nitrogen (N).

114 **2.** Methods

115 2.1. THE INVEST NUTRIENT DELIVERY RATIO MODEL

116 The InVEST (v.3.3.3) suite of tools has been developed to enable decision makers to assess trade-offs

across ecosystem services and to compare the consequences of different future change scenarios,

118 for example in land use or climate (Sharp et al. 2016). To this end, InVEST comprises a set of models

that cover a wide range of ecosystem services. Like many ecosystem service models, these models
are based on comparatively simple production functions, enabling them to be run quickly on a
standard desktop computer and to take advantage of readily available data (Sharp et al. 2016) and
targeting a user community with potentially limited technical background.

123 The UK has a long history of issues arising from nutrient contamination of watercourses (Johnes et 124 al. 1996; Withers and Lord 2002), as it is densely populated and has a large proportion of its land 125 area under anthropogenic land uses (i.e. agricultural and urban land). This results in high levels of 126 nutrient input to freshwater systems, and ensuing concerns over the contamination of drinking 127 water and damage to aquatic ecosystems via eutrophication (Withers and Lord 2002). Validated 128 nutrient export models, with clear estimates of their accuracy and uncertainty are therefore 129 particularly valuable to compare nutrient exports under different scenarios of environmental change 130 or management interventions over larger spatial scales (Johnes et al. 1996; Shepherd et al. 1999; 131 Wilby et al. 2006).

The InVEST nutrient delivery ratio (NDR) model aims to quantify relative nutrient export and retention across different catchments or sub-catchments, and to reflect changes in nutrient export/retention under different change scenarios. The model maps the transport of nutrients from catchment sources to the stream network. It combines the advantages of nutrient transport models (e.g. SWAT (Arnold et al. 1998); RHESSys (Tague and Band 2004)), which often work at the scale of subwatersheds or hydrological units to provide quantitative estimates of nutrient flows, and index models (Drewry et al. 2011), which spatially map source risk and transport factors.

The model computes a nutrient mass balance that represents the long-term, steady-state flow of 139 140 nutrients based on i) nutrient sources associated with different land use/land cover (LULC) in the 141 landscape, and ii) the retention properties (e.g. LULC, slope) of pixels belonging to the same flow 142 path (Parn et al. 2012; Sharp et al. 2016). Specifically, nutrient sources across the landscape are 143 derived from LULC-specific nutrient application (loading) rates, which can be determined from 144 empirical data. Nutrient sources can be divided into surface and subsurface sources (which 145 conceptually represent sediment-bound and dissolved components, a distinction common to many 146 nutrient transport models (Newham et al., 2004; Newham et al., 2008). The model only includes 147 diffuse sources of nutrient; point sources are not included and need to be added in post-processing of model outputs. Next, the model uses topographic routing and an index, the NDR factor, to 148 149 emulate the movement of nutrients across the landscape and into a watercourse. The NDR factor is 150 calculated for each landscape pixel based on the properties (e.g. slope, retention coefficient) of 151 pixels that belong to the same flow path. This empirical approach is in contrast to more complex,

process based models that incorporate detailed representations of nutrient cycling (see Breuer et al. 152 153 2008 for a review). At the catchment outlet, the nutrient export to water is calculated as the sum of 154 the pixel-level contributions. For further details on the model, see Supplementary Material, 155 Appendix S1 and Sharp et al. (2016). Model source code is available in Hamel and Sharp (2017) 156 Because of the qualitative nature of the NDR factor approach, calibration of the model is necessary 157 to gain confidence in the quantitative outputs. The main calibration factor is the k_b parameter, which 158 governs the relationship between the connectivity index, which is a function of topography, and the 159 NDR factor. This relationship is further described in the user's guide (Sharp et al., 2016) and is akin to 160 the structure of the InVEST sediment delivery ratio model (Hamel et al. 2015), which can be used

161 independently to model this other facet of water quality.

162 2.2. MODEL INPUTS

Spatially explicit model inputs required for the NDR model are a digital elevation model (DEM), land 163 164 use/land cover (LULC) raster data, nutrient runoff proxy raster data and a vector delineation of the watersheds. We used the Centre for Ecology & Hydrology's Integrated Hydrological Digital Terrain 165 Model (CEH IHDTM, Morris and Flavin 1990) for the DEM. The IHDTM was resampled or aggregated 166 167 to the required resolution (see below), filled to eliminate sinks and combined with a digital 168 watercourse network (Moore et al. 1994) to ensure routing along known watercourses. These 169 processes were performed in ArcMap (v10.3 © ESRI, Redlands, CA). The model also requires a 170 threshold value for flow accumulation (TFA) to define streams, which is expressed as a number of 171 upstream pixels. Within the model, watercourses are assumed not to retain or add to the nutrient 172 load, and nutrients reaching a stream pixel will contribute directly to the total load from the 173 catchment (Sharp et al. 2016). The TFA value was selected following sensitivity analyses and 174 examination of watercourse maps (See below, section 2.3).

175 LULC data were obtained from the 25 m resolution raster version of the UK Land Cover Map 2007 176 (LCM2007, Morton et al. 2011). The LCM2007 data are derived from satellite imagery, generalised 177 digital cartography and image segmentation, and classify the UK land surface into 23 broad habitat 178 classes (Jackson 2000; Morton et al. 2011). The InVEST model requires several parameter values for each distinct LULC class. These include the nutrient load applied to the land (kg ha⁻¹y⁻¹), the 179 180 proportional retention of that nutrient load, the length of flow path required to achieve that 181 retention (in metres), and the proportion of the nutrient load that travels via subsurface flow. This 182 last variable is set to zero by default, making the assumption that all nutrients travel via surface or shallow subsurface flow. However, if modified, the model then requires two further parameters -183 184 the subsurface nutrient retention efficiency and the flow length required to achieve this.

185 Nutrient loading and nutrient retention coefficients for each LULC class were obtained by performing 186 an extensive literature search for values relevant to the UK and for habitats that most closely 187 matched the broad habitats defined by the LCM2007 (Supplementary Material, Table S1). Where 188 several possible values for a single LULC class were found, the median value was used. A wide variety 189 of sources provided information on P (Dillon and Kirchner 1975; Fozzard et al. 1999; Johnes 1996; 190 May et al. 2001; May et al. 1996; McGuckin et al. 1999; Smith et al. 2005) with rather fewer 191 supplying suitable values for N (Johnes 1996; Shi et al. 2006). Because many of these publications 192 report measured or estimated export coefficients from land to water, which are a function of the 193 two required model inputs (load to land and retention), some loads were estimated from export 194 coefficients according to the following formula (Sharp et al. 2016):

195 $Load to land = \frac{Export from land}{1 - Retention}$

Critical flow length (i.e. the distance of travel required to achieve the nutrient retention coefficient)
was set to the resolution of the input LULC raster across all LULC classes, catchments and nutrients,
which was consistent with the relatively coarse resolution (25m at the minimum).

199 Previous studies have shown that choice of input data can have major impacts on the accuracy of 200 InVEST ecosystem service models where these data relate to parameters to which the model is 201 highly sensitive (Hamel and Guswa 2015; Pessacg et al. 2015; Redhead et al. 2016; Sánchez-Canales 202 et al. 2012). We compared three sets of input data for the nutrient runoff proxy raster. These were, 203 1) WorldClim precipitation data (Hijmans et al. 2005), which are readily available, widely used and 204 have global coverage interpolated to approximately 1km resolution 2) UK Met Office UKCP09 data at 205 5km resolution (Jenkins et al. 2008; Perry and Hollis 2005), which gave good estimates of total 206 annual water yield when used in the relevant InVEST model (Redhead et al. 2016), and 3) CEH-GEAR 207 data at 1km resolution (Tanguy et al. 2014), which has a higher spatial resolution. All datasets 208 comprise gridded rainfall per raster cell at monthly or annual time steps, derived from interpolation 209 and correction for geographic and topographic factors of measurements taken from a national 210 network of meteorological stations. Data were derived from the mean of annual values between 211 2000 and 2012 to match the period of the validation data. We also tested a randomised dataset 212 using values drawn from the range of all three datasets to test the impact of large errors in the 213 nutrient runoff proxy raster on model accuracy.

214 2.3. SENSITIVITY ANALYSIS

As well as varying input datasets for the nutrient runoff proxy raster we also tested the sensitivity of the model to changes in the values of the input parameters. This is key to understanding why the

217 model behaves as it does, setting appropriate ranges for calibration of parameter values and helping 218 subsequent users to identifying those parameters for which it is most worthwhile investing in to 219 obtain more accurate data. To do this, first we ran the model on "hypothetical" versions of our test 220 catchments, with the UKCP09 precipitation data, default values for threshold flow accumulation and 221 k_b parameter (TFA = 1000 and k_b = 2, respectively), input LULC and DEM raster resolution of 25m and 222 a single land cover class with a mean nutrient load to land (4.7 kg ha⁻¹y⁻¹) and retention (0.3) 223 (because the model has the same structure, these analyses are valid for N and P). We then varied 224 each of the precipitation data, nutrient load and nutrient retention by ±50% and ±90% and examined 225 the percentage difference in modelled nutrient export to water. These values were chosen because 226 the percentage difference between the median and maximum/minimum export coefficients was 227 approximately 100%, so these variations explore the likely range of variation encountered when 228 using literature derived coefficients.

229 For the single-value parameters (TFA and k_b) we explored a range of values. We tested three TFA 230 values (100, 1,000 and 10,000). We used these three values because preliminary analyses 231 determined that more subtle variations in TFA made very little difference to the overall length of 232 steam network, especially in larger catchments. Preliminary analyses also determined that values 233 below 100 were very likely to overestimate the stream network density, whilst values above 10,000 234 were not met in all catchments (i.e. no modelled watercourses were created). Because the ideal TFA 235 value was catchment specific (see Results, section 3.1), we also used another approach, which 236 involved setting the threshold either at default (1000) or high (10,000) but combining known 237 watercourses into the LULC raster as a separate class with appropriately low retention. We used the 238 same digital watercourse network to do this as was used to correct the flow paths generated from 239 the DEM (Moore et al. 1994). For k_b we compared values of 0.5, 1, 2 (the default), 4, 8 and 16. 240 Preliminary analyses determined that, whilst k_b is dimensionless and can in principle accept any 241 value, values above this range made progressively less differences to the relationship between 242 topography and nutrient delivery, whilst values below this range tend to collapse the function to the 243 point where extreme changes in connectivity are required to impact on nutrient delivery. In all model runs we assumed a subsurface flow proportion of zero (i.e. all nutrient transported via 244 245 surface flow).

Because the spatial scale and resolution of the input data can affect ecosystem service model
outputs (Sharp et al. 2016), especially those with a dynamic flow component (Grafius et al. 2016), we
also compared models run with versions of the LCM2007 and IHDTM at the highest resolution
available (25m, the resolution of the raster LCM2007), and at lower resolutions that could easily be
derived from these data (50m, the resolution of the IHDTM, 100, 200, 400 and 800 m.) Coarser

resolutions greatly speed up the modelling but potentially reduce accuracy. When changing the
resolution of the input rasters, TFA was adjusted to keep the flow path length consistent across
raster resolutions, following Hamel et al. (2017). Coarser inputs than 800m were not tested, as at
values above this some smaller catchments begin to have flow paths of only 1 or 2 cells, making
setting an appropriate TFA impossible.

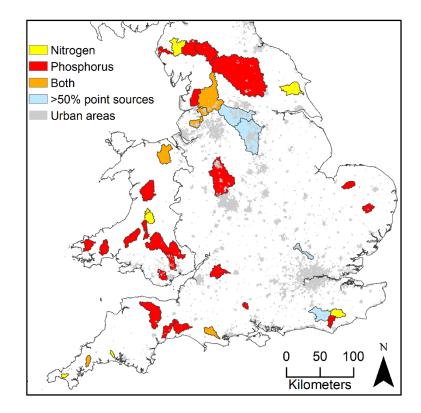
256 2.4. VALIDATION DATA

The data used for validation were derived from the UK Environment Agency's Water Information 257 258 Management System (WIMS), which provides records of total N and total P concentrations for a 259 network of sampling points across England and Wales (Envrionment Agency 2017). Because these 260 data represent instantaneous concentrations of nutrients, it was necessary to find sites with 261 coincident records of river flow, and sufficiently frequent measurements of nutrient concentrations 262 to enable the robust estimation of total annual nutrient load in the watercourse - comparable with 263 the output of the NDR model – and to account for inter- and intra- annual variation. To achieve this, 264 sites from WIMS were filtered to exclude sites with less than 5 years of available data over the years 265 2000-2010, with each year containing at least one measurement per month of total N or P. These 266 sites were then overlain with the locations of all flow gauging stations in the National River Flow 267 Archive (NRFA). The NRFA collates, quality controls, archives and disseminates hydrometric data 268 from gauging stations operated by government funded environmental bodies across the UK (Fry and 269 Swain 2010). WIMS sites that were spatially coincident with NRFA gauging stations had the 270 necessary daily flow data available to enable annual nutrient loads to be calculated and their 271 catchments had been previously defined using the IHDTM. These temporal and spatial filters 272 resulted in 33 catchments being identified as having sufficient data to act as a validation dataset for 273 P. However, because total N was measured at a smaller proportion of sites (most measure NOx), 274 only three catchments met all of the above criteria for N. Therefore, we reduced to three the 275 required number of years with at least monthly measurements, giving 16 catchments with sufficient 276 data for N.

277 Total annual nutrient load for each year was calculated from the WIMS and NRFA data for each 278 catchment using the Beale Ratio Estimator (BRE, Beale 1962) which relates the ratio of average load 279 to average flow, at times when concentrations are measured, to the ratio of average true load to 280 average true flow over the entire period of interest (Dunn et al. 2014). Whilst there are a wide 281 variety of methods available with which to extrapolate loads from intermittent data, ratio estimators 282 have been used in previous validation studies (Terrado et al. 2014) and the BRE has been shown to 283 produce robust results, especially when the measurement frequency of the concentration data is 284 lower than that for discharge (Dolan et al. 1981; Dunn et al. 2014; Meals et al. 2013; Quilbé et al.

285 2006; Richards and Holloway 1987), as was the case here. The median BRE nutrient load across286 years for each catchment was then calculated.

287 Because the NDR model only accounts for nutrients from diffuse sources, it was necessary to adjust 288 the modelled output of total load by an estimated load for point sources, to enable comparison with 289 the validation data. In the UK, point sources can contribute the majority of P and a substantial 290 proportion of N to waterways (Edwards and Withers 2008), although this varies across space and 291 time (Arheimer and Lidén 2000). The estimated load from point sources was obtained using a GIS 292 layer of wastewater treatment works (WWTWs) provided from UK Water Companies through the 293 Environment Agency (see Williams et al. 2009). Although there is a wide variety of other point 294 sources of N and P releases (Edwards and Withers 2008), WWTWs are likely to be the largest 295 contributor at a whole-catchment scale in the UK (Bowes et al. 2005; Edwards and Withers 2008). 296 For each WWTW, data were available describing the maximum human population served and the 297 treatment type employed (i.e. primary, secondary or tertiary). These data were combined with a 298 mean annual per capita export of P and N in untreated sewage of 0.52 kg P and 4.5 kg N and nutrient 299 retention efficiencies for the different treatment types, both derived from a recent UK-wide review 300 (Naden et al. 2016), to give an estimated annual N and P output for each WWTW. N and P outputs 301 from individual WWTWs were then summed to give an annual load from WWTWs per catchment. 302 This value was then subtracted from the per-catchment BRE to give a total export from diffuse sources only for comparison with the output of the InVEST NDR model. We removed catchments for 303 304 which the estimated nutrient export from point sources contributed to more than 50% of the total 305 estimated export (mostly relatively heavily urbanised catchments, Fig. 1), as these were unlikely to 306 be well represented by the model (which focuses on diffuse sources) and would be highly influenced 307 by any errors in our estimation of point source nutrient exports, giving final sample sizes of 28 for P 308 and 14 for N (Figure 1 and Supplementary Material, Table S1).



309

Fig. 1. Map of southern UK showing catchments providing validation data for nitrogen (yellow),
phosphorus (red) or both (orange). Blue catchments indicate those which had sufficient nutrient
and flow measurements, but were estimated to have over 50% of total nutrient runoff due to point
sources and so were excluded from further analyses. Urban areas are also shown in grey (from
LCM2007). Note that none of these catchments overlap.

315 2.5. STATISTICAL ANALYSIS

Comparisons between the modelled and measured data were made by performing linear regressions
implemented in R (R Core Team 2014), as well as comparing the percentage differences between
modelled and measured. Many stakeholders require models simply to predict accurately the rank
order of locations in terms of ecosystem services, rather than absolute values (Willcock et al. 2016)
and the InVEST model does not necessarily aim for accurate prediction of values (Sharp et al. 2016).
Therefore, we also tested the accuracy of the InVEST NDR model in predicting relative export values
using rank correlation (Spearman's rho).

323

324 **3.** Results

325 3.1. SENSITIVITY ANALYSIS

- 326 Modelled nutrient export from the NDR model was insensitive to variation in precipitation
- 327 (Supplementary Material Fig S1A). This was expected since these variations were applied as

consistent percentage change across the entire spatial extent. Because the role of this input is to
represent relative runoff between pixels, the model is still likely to be sensitive to different inputs
where they show different spatial patterns, as opposed to different magnitudes. This was addressed
by comparing the three different input datasets (see below, Section 3.2).

The model was sensitive to variation in the nutrient loading and retention values (Supplementary
 Material Fig S1B and S1C) although sensitivity was linear. Because land cover was held constant for
 these analyses, sensitivity to these parameters did not show any catchment specificity.

- 335 In contrast, sensitivity to the two calibration parameters was highly catchment specific. Figure 3
- 336 illustrates the percentage change in modelled nutrient export compared to the values obtained
- 337 when using the default parameter values of 2 for k_b and 1000 for TFA. The effect of k_b on the
- 338 magnitude and direction of change in nutrient export was catchment specific (Fig 2A). Overall,
- decreasing k_b to 0.5 produced the most extreme changes (-20% to +35%), whilst increasing k_b to 4
- resulted in changes of $\pm 10\%$. Further increases in k_b resulted in changes that remained within this
- range for the majority of catchments (Fig 2A). Catchment sensitivity appeared driven by topography,
- 342 with more topographically varied catchments in the uplands showing decreases in nutrient export in
- response to increased k_b values and less varied, lowland catchments showing the opposite response
- 344 (Pearson's *r* against % change at $k_b = 0.5$; Mean catchment altitude n = 35, r = 0.704, p < 0.001;
- Standard deviation in catchment altitude n = 35, r = 0.709, p < 0.001).

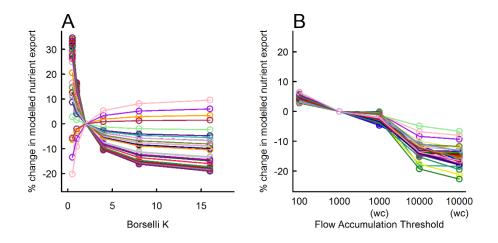


Fig. 2 Sensitivity of the NDR model output to variation in the values of A) Borselli k_b parameter and
B) Flow accumulation threshold, TFA (with wc indicating where the threshold was applied along with
known watercourses from the digital watercourse network being added to the LULC raster). Each
colour represents a different catchment.

- 351 Sensitivity to variation in the flow accumulation threshold TFA was also catchment specific (Fig 2B).
- 352 This was unsurprising as the degree to which a given TFA value accurately represents actual

353 watercourses will vary among catchments depending on their hydrogeology and topography. As can be seen in Figure 4, the default value of 1000 overestimated the stream density in some catchments 354 355 whilst underestimating it in others. Thus, either reducing or increasing the threshold improved 356 representation of the routing of nutrients in some catchments but made it less accurate in others -357 values of 100 captured most watercourses in some catchments (Fig. 3A and 3B) whilst in others 358 actual watercourses were best represented by TFA of 10,000 (Fig. 3C and 3D). Addition of mapped 359 watercourses to the LULC input with a TFA of 1000 resulted in comparatively minor changes to the 360 nutrient export (Fig 2B), but ensured that no catchment had known watercourses which were not 361 modelled as such. Using the same approach with a TFA of 10,000 had a large effect on the modelled 362 nutrient export (Fig 2B), reducing nutrient export by up to 20%, by restricting in-stream transport to 363 mapped watercourses only. Which of these latter results is the more accurate is likely to depend on 364 the accuracy of the mapped watercourse network (Baker et al. 2007), many of which, for example 365 ditches and field drains, have not been mapped into a hydrologically consistent network for the UK. 366 Because small, unmapped watercourses are known to have a potentially high impact on nutrient flux 367 (Edwards and Withers 2008; Foster et al. 2003; Heathwaite et al. 2006) we chose to use a TFA value 368 of 1000 with watercourses from Moore et al. (1994) added to the LULC raster for further analyses.

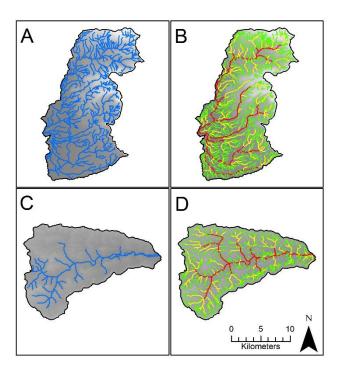


Fig. 3 Examples of two catchments showing the catchment specific effects of variation in the flow
accumulation threshold, TFA, on modelled watercourse location. Panels A and C show the known
watercourse network (in blue) overlain onto the hydrologically corrected digital elevation model.
Panels B and D show streams as determined by three flow accumulation thresholds (100 = green;

374 1000 = green + yellow; 10,000 = green + yellow + red). The catchments are shaded according to
375 altitude from dark (low, minimum = sea level) to pale (high, maximum = 600 m.a.s.l) grey.

376 3.2. MODEL VALIDATION AND COMPARISON OF INPUT DATASETS

377 Whilst the slope of the relationship remained similar for both nutrients, both N and P showed 378 increasing percentage differences at resolutions coarser than 100m (Table 1 and Figure 4A and D). 379 When reporting percentage differences across catchments we used the median of mathematical 380 absolute percentage differences to avoid spurious impressions of increased average accuracy 381 resulting from a wider range of under- and overestimates. At coarser (>100m) resolutions, although 382 absolute values became increasingly erroneous for both nutrients, modelled N tended to preserve 383 relative magnitudes of differences between catchments (shown by slightly increased Spearman's ρ). 384 Indeed, the relatively stable values for r_{LR}^2 for N suggest that coarser resolutions gave increasingly 385 severe underestimates, but that the relationship between modelled and measured data remained 386 relatively consistent across catchments. In contrast, at coarser resolutions than 100m, modelled P 387 became increasingly inaccurate in terms of both absolute and relative export, and the relationship 388 between modelled and measured data became increasingly inconsistent (table 1).

389 In practical terms, finer resolutions substantially increased the model run time, from around 30 390 seconds at 800m resolution, through 5 minutes at 100m resolution to around 4 hours at 25m 391 resolution. The size of the input and output files was also substantially greater at finer resolutions, 392 with output export maps for a single nutrient of 1.5 gigabytes, 100 megabytes and 2 megabytes for 393 resolutions of 25, 100 and 800 metres, respectively. Given the observed drop off in r_{LR}^2 and 394 Spearman's ρ for P and the increased percentage difference between modelled and measured data 395 for both nutrients at resolutions coarser than 100m (Table 1 and Figure 4) we selected a resolution 396 of 100m for further model testing and validation.

Table 1 Comparisons of total P and N export from the InVEST NDR model with exports estimated from measured flows and nutrient concentrations, for varying resolutions of input data. Estimated exports were adjusted to remove point sources. Results are: median absolute percentage difference; Spearman's ρ and the intercept, slope and $r^2 (r_{LR}^2)$ of a linear regression; between the two datasets.

		Median	с <i>і</i>	Linear regression		
Nutrient	Resolution (m)	absolute % difference	Spearman's rho (ρ)	Intercept	Slope (± 95% Cl)	r _{LR} ²
hor	25	54.51	0.77	0.31	0.49 (±0.12)	0.72
Phosphor us	50	56.43	0.78	0.34	0.49 (±0.12)	0.71
노	100	55.73	0.79	0.34	0.49 (±0.12)	0.73

	200	56.30	0.79	0.31	0.48 (±0.13)	0.69
	400	67.91	0.75	0.15	0.47 (±0.14)	0.62
	800	88.96	0.56	-0.28	0.44 (±0.23)	0.36
	25	72.57	0.75	0.31	0.67 (±0.27)	0.71
-	50	70.37	0.78	0.33	0.67 (±0.27)	0.72
Nitrogen	100	72.58	0.81	0.28	0.69 (±0.25)	0.76
Nitr	200	76.56	0.83	0.15	0.71 (±0.23)	0.80
	400	84.11	0.87	-0.25	0.79 (±0.23)	0.81
	800	95.51	0.88	-1.28	0.98 (±0.37)	0.73

402

403 Because the sensitivity of the model to k_b appeared relatively high (Fig. 3A), and because there was 404 no clear way to assess which value was most appropriate from our sensitivity analysis alone, we ran 405 the model and compared to validation data for values of k_b of 0.5, 1, 1.5, 2, 2.5, 3, 3.5 and 4. We did 406 not explore values of k_b beyond the range 0.5 - 4 here because sensitivity analysis demonstrates that 407 at values much over 4 the impact of Kb on the model levels off, whilst at values approaching zero, 408 the results diverge towards extreme values (Figure 2A). Overall, the effect of varying k_b on the fit to 409 the validation data was not large, with near identical r_{LR}^2 , slope and Spearman's correlation 410 coefficient (Table 2). From Figure 4B and 4E, it can be seen that lower k_b values resulted in median 411 percentage differences closer to zero, but this appears due to an increased number of outliers with 412 substantial overestimates rather than a general improvement across catchments. This is perhaps 413 unsurprising, given the widely varying catchment responses to changes in k_b seen in Figure 3A. There 414 was thus no clear evidence to support altering the value of k_b from the default of 2 for our modelling 415 across multiple catchments.

Table 2 Comparisons of P and N export from the InVEST NDR model with exports estimated from
measured flows and nutrient concentrations (adjusted to remove point sources), for eight values of

	-	Median	Spearman's rho (ρ)	Linear regression		
Nutrient		absolute % difference		Intercept	Slope (± 95% Cl)	r _{LR} ²
	0.5	41.16	0.77	0.41	0.49 (±0.12)	0.71
Phosphorus	1	53.97	0.76	0.37	0.49 (±0.12)	0.71
	1.5	58.43	0.77	0.33	0.49 (±0.12)	0.71
	2	55.73	0.79	0.34	0.49 (±0.12)	0.73
	2.5	56.99	0.79	0.32	0.49 (±0.12)	0.72
	3	55.41	0.79	0.31	0.49 (±0.12)	0.72
	3.5	53.59	0.79	0.30	0.49 (±0.12)	0.72

_	4	54.54	0.79	0.29	0.49 (±0.12)	0.72
	0.5	64.00	0.78	0.38	0.68 (±0.24)	0.75
	1	72.99	0.78	0.32	0.68 (±0.24)	0.75
-	1.5	75.49	0.80	0.27	0.68 (±0.24)	0.76
Nitrogen	2	72.58	0.81	0.28	0.69 (±0.25)	0.76
Nitr	2.5	73.72	0.81	0.25	0.69 (±0.25)	0.76
	3	74.52	0.81	0.22	0.70 (±0.25)	0.76
	3.5	75.11	0.81	0.21	0.70 (±0.25)	0.76
	4	75.56	0.81	0.19	0.70 (±0.24)	0.77

419

420 Having explored the effect of k_b and the input data resolution, we then compared the three input

421 precipitation data sources. The choice of precipitation data again made comparatively little

422 difference to either N or P export (Table 3 and Figure 4C and 4F). The randomised precipitation

423 dataset did show reductions in ρ and r_{LR^2} but actually decreased median percentage difference.

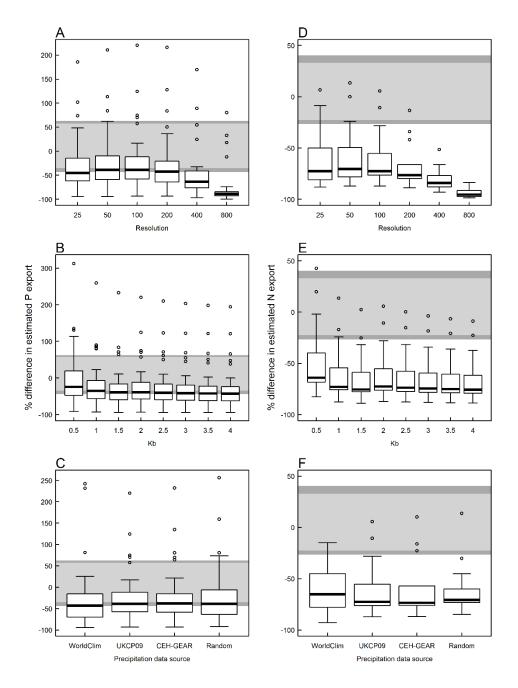
424 Table 3 Comparisons of total P and N export from the InVEST NDR model with exports estimated

425 from measured flows and nutrient concentrations (adjusted to remove point sources), for three

426 difference sources of precipitation data (WorldClim, Met Office UKCP09 and CEH-GEAR).

	Precipitation data source	Median absolute % difference	Spearman's rho ($ ho$)	Linear regression		
Nutrient				Intercept	Slope (± 95% Cl)	<i>r</i> _{LR} ²
S	WorldClim	56.40	0.81	0.33	0.51 (±0.12)	0.73
horu	UKCP09	55.73	0.79	0.34	0.49 (±0.12)	0.73
Phosphorus	CEH-GEAR	57.07	0.77	0.35	0.49 (±0.12)	0.71
	Random	55.13	0.69	0.37	0.46 (±0.17)	0.53
	WorldClim	70.70	0.88	0.17	0.74 (±0.21)	0.83
Nitrogen	UKCP09	72.58	0.81	0.28	0.69 (±0.25)	0.76
	CEH-GEAR	73.59	0.84	0.28	0.69 (±0.25)	0.75
	Random	65.27	0.74	0.28	0.68 (±0.27)	0.71

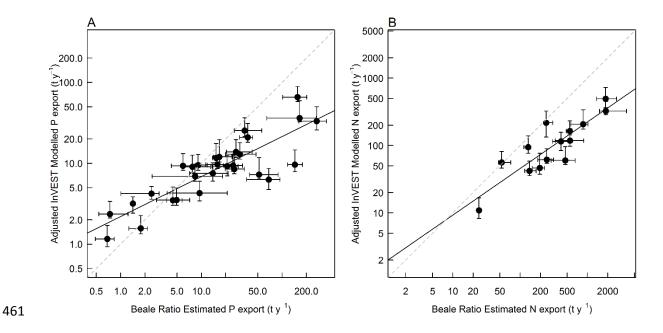
427



430

Fig. 4 Boxplots showing the effect of spatial resolution (i.e. dimensions of raster cells in metres) 431 (A,D), Borselli k_b (B,E) and precipitation data source (C,F) on percentage differences between 432 estimated total nutrient export per catchment from the InVEST NDR model and corresponding 433 434 exports estimated from gauged flow and measured nutrient concentration data (adjusted to remove 435 point sources), for phosphorus (A,B,C) and nitrogen (D,E,F). Grey shaded areas indicate the range of 436 variation in estimated nutrient export values resulting from interannual variation in estimated 437 exports (quartiles, light grey) and the maximum and minimum values for average per capita nutrient 438 outflow from point sources (dark grey)

- 439 Modelled total nutrient export showed a better fit to the empirical data than did modelled load 440 alone (P: $r_{LR}^2 = 0.73$, 0.56, Spearman's $\rho = 0.79$, 0.69, N: $r_{LR}^2 = 0.76$, 0.72, Spearman's $\rho = 0.80$, 0.75, 441 for load and export, respectively, with 100m resolution inputs, $K_b = 2$ and UKCP09 precipitation 442 data). The NDR factor component of the model thus results in substantial increases in model 443 performance over a simple summation of loads, especially for P.
- 444 Because the results at all values of k_b and the different precipitation datasets resulted in good predictions of the relative magnitude of nutrient export ($\rho = 0.77 - 0.81$ and 0.75 - 0.88, for 445 446 phosphorous and nitrogen, respectively) but relatively large underestimates of absolute values 447 (range of absolute median estimates $\pm 44.4\% - \pm 58.4\%$ and $\pm 65.3\% - \pm 76.6\%$ for phosphorous and 448 nitrogen, respectively), we ran a final model with reduced retention coefficients for both nutrients. 449 Whilst this deviates from parameter values reported from empirical studies (see section 2.2), we 450 were interested to see if a large improvement in accuracy could be made by performing a simple, 451 uniformly applied adjustment to retention values. We therefore divided retention values by two and 452 re-ran the model (with 100m resolution inputs, $K_b = 2$ and UKCP09 precipitation data). Although this resulted in slightly reduced absolute median percentage differences (by 8.5% and 9.2% for 453 454 phosphorous and nitrogen, respectively), the Spearman's ρ and the slope and r_{LR}^2 from linear 455 regression were also reduced (4-10% reduction Spearman's ρ , 4-13% reduction in r_{LR}^2 , 8%-12% 456 reduction in slope). This suggests that modifying the retention coefficients away from literature 457 values helps to reduce the median level of underestimates, but reduces the ability of the model to predict relative magnitude of nutrient export between catchments, probably by worsening 458 459 overestimation in low exporting catchments whilst improving underestimation in high yielding ones 460 (Figure 5).



462 Fig. 5. Nutrient export per catchment from the InVEST NDR model plotted against exports estimated 463 from measured flows and nutrient concentrations (adjusted to remove point sources), for P (panel A) and N (panel B). Points represent InVEST results (input resolution = 100m, k_b = 2, precipitation 464 465 data = UKCP09) against Beale Ratio Estimated nutrient export from measurements. Horizontal bars span the range given by 25th to 75th percentile of interannual variation in the Beale ratio estimated 466 467 nutrient export ± the maximum and minimum values for average per capita nutrient outflow from point sources. Vertical bars indicate the range in modelled export resulting from running the model 468 469 with values of k_b between 0.5 and 4, input raster resolution of 25, 50, 100 and 200 metres and the 470 three different precipitation datasets. A 1:1 relationship is indicated by the dotted line. Note axes 471 are on a log10 scale.

472 **4.** Discussion

473 4.1. PERFORMANCE OF THE INVEST NDR MODEL

474 Our results suggest that the InVEST NDR model can give good results in terms of the relative 475 magnitude of N and P export across a wide variety of UK river catchments, with ρ between 0.7 and 476 0.83 depending on the scale of input data and parameter values used. However, accuracy in terms 477 of estimating actual nutrient export was comparatively low with the majority of catchments showing 478 over or underestimates of up to 44% for P and 65% for N. It should be noted that attempting to gain 479 good model performance over a large number of widely varying catchments is a challenging test for 480 the model. Performance is expected to be higher with calibration at the regional level with catchments having similar hydrogeological properties. Whilst some studies perform such model 481 482 performance assessment (e.g. Bai et al. 2013; Terrado et al. 2014), many ecosystem service models 483 are applied at regional or national scales without validation (Martínez-Harms and Balvanera 2012). A 484 survey across sub-Saharan Africa demonstrated that many stakeholders wish to run ecosystem 485 service models at national scales (Willcock et al. 2016). Furthermore, ecosystem service models are 486 often perceived as being of great use in data-scarce parts of the world (Pandeya et al. 2016; Villa et 487 al. 2014) where there are few opportunities to calibrate or validate. Therefore, it is important for 488 studies such as ours to demonstrate some of the possible pitfalls of applying ecosystem service 489 models without extensive validation and sensitivity testing.

490 4.2. UNDERSTANDING MODEL SENSITIVITIES

Sensitivity to variation in the input parameter values is unsurprising and, of course, desirable if a
model is to be used to assess change over time or among future change scenarios. However, it is
also important to understand that such sensitivities can determine how appropriate a model is to a
particular study region, where to focus most effort on data acquisition (Boithias et al. 2014; Sánchez-

Canales et al. 2012), or to aid in assessing the uncertainty associated with model outcomes. In brief,
the model appeared most sensitive to the nutrient loading and retention values, the threshold flow
accumulation and the resolution of the input raster data (beyond a certain range). We discuss each
of the parameters in turn.

499 4.2.1. Nutrient load and retention

500 The linear response between nutrient export and nutrient load and nutrient retention coefficients is 501 to be expected, given that nutrient export is calculated as the product of nutrient load on a pixel and 502 the NDR factor, which is proportional to nutrient retention parameters from downslope pixels. 503 These parameters are thus the major drivers by which the spatial configuration of land use/land 504 cover affects nutrient runoff. Importantly, nutrient loads and retention efficiencies will vary greatly 505 in time and space. In our test catchments, most of which are dominated by arable land or 506 agriculturally-improved grassland, such variation will be driven by crop type, stocking density, 507 fertiliser application rates and timings, and other farm management practices. It is, therefore, 508 essential to research these values sufficiently to ensure that they are robust for the land cover types 509 that are dominant in the study region and those that are of most interest in relation to any change 510 scenarios that are being explored.

511 4.2.2. *k*^b parameter

512 The Borselli k_b parameter determines the relationship between hydrologic connectivity (the degree 513 of connection from patches of land to the stream) and the NDR. Higher values mean that the 514 relationship between the connectivity index and the NDR factor becomes linear, whereas lower 515 values mean that this relationship becomes a step function. This relationship is site-specific, as 516 demonstrated by the very different responses to varying k_b shown by different catchments in our 517 sensitivity analysis. This is also likely to be the reason that, from our results, calibration to produce 518 the best cross-catchment absolute accuracy may not result in the most accurate predictions of 519 relative magnitude between catchments and vice versa. Therefore, although this parameter is in 520 practice the main parameter used for calibration (Sharp et al. 2016), where possible k_b should be 521 determined regionally, across catchments with similar hydrogeological properties.

522 4.2.3. Threshold flow accumulation

523 Varying the flow accumulation threshold TFA had a substantial effect on model output. This effect is

524 partly explained by the model structure, which assumes that stream pixels do not export any

- nutrient. Therefore, changing the density of the stream network also changes the number of pixels
- that actually contribute to nutrient loading and retention (e.g. 66%, 92%, 98%, 99% at TFAs of 10,
- 527 100, 1000 and 10000, respectively, at 25m DEM resolution). Our results show that, as with k_b ,

selecting a single value that is equally applicable across a number of catchments is difficult, because
catchment topography and hydrogeological attributes (e.g. groundwater flow) can change the
threshold that needs to be set to capture actual watercourses. Comparing the derived stream
network to a known watercourse network is a key first step to selecting an appropriate value, and
our results also suggest that modifying the DEM and LULC map to capture known watercourse
networks may provide a robust approach to overcoming this issue when conducting cross-catchment
analyses.

535 4.2.4. DEM and LULC raster resolution

536 Changing the resolution of the input DEM and LULC spatial data had comparatively little effect on 537 the accuracy of the model output for both P and N at resolutions less than or equal to 100m. Whilst 538 this is in contrast to other studies which have concluded that increased data resolution usually 539 results in increased model accuracy (Brazier et al. 2005), decreased sensitivity to input raster 540 resolution is a stated aim of the design of the NDR model (Sharp et al. 2016), hence the inclusion of 541 TFA and critical flow length parameters which the user can modify. It appears that resolutions finer 542 than 100m gain little in absolute accuracy to justify the very substantial increases in file size (making 543 data harder to store, manage and disseminate) and running time which result from running the 544 model with finer resolution inputs.

545 However, resolutions coarser than 100m resulted in decreasing accuracy, especially for P. This is 546 likely to be a result of coarser resolution cells losing spatial detail, with values being generalised to 547 average (DEM) or dominant (LULC) values per cell. The most likely mechanism for the effects we 548 observed are loss of detail from the LULC raster. If the key LULC classes governing nutrient export 549 are relatively small in area, they may be lost from aggregated inputs. For example, in UK upland 550 catchments which are largely semi-natural, small areas of agricultural land close to watercourses 551 would have a disproportionate effect on total nutrient export, but may not form the majority cover 552 of any non-watercourse pixels in a coarse resolution LULC map, removing their potential to influence 553 modelled nutrient export. The two nutrients differed somewhat in their responses to resolution 554 (with N retaining accurate relative magnitude and a consistent relationship between modelled and 555 measured data, even though underestimation became more severe). This is probably because of their different loadings and export pathways. Phosphorus is more associated with high releases from 556 557 proportionally small areas with high hydrologic connectivity whilst nitrogen is more evenly spread 558 across land cover classes and less directly linked to the degree of hydrologic connectivity (Edwards 559 and Withers 2008; Withers and Lord 2002), such that the loss of spatial detail at coarser resolutions 560 affects the ability of the model to reflect actual export to different degrees.

561 4.2.5 Precipitation data source

562 Unlike the InVEST water yield model (Redhead et al. 2016), the NDR model appeared relatively 563 insensitive to the source of input precipitation data. All three datasets produced similar results, and 564 even the randomised data only reduced accuracy slightly. To some extent this is unsurprising. The 565 effect of precipitation data is to modify the per pixel load to account for runoff potential by relating 566 the precipitation per cell to the average across the raster (see Supplementary Material, Appendix 567 S1). Therefore, providing that general spatial patterns are preserved between input datasets, this 568 should be sufficient to obtain similar results. The lack of effect of using randomised data is perhaps 569 more surprising, as here the spatial pattern of relative runoff has been removed. However, by using 570 long term average data at 1km to 5km scales, the range of values is not high within many 571 catchments, so even when randomising the data the distribution of runoff potential across the 572 landscape does not vary hugely (Supplementary Material, Table S2). Of course, for those catchments 573 with a higher range in precipitation (in our analysis this was limited to larger catchments spanning 574 upland and lowland), randomisation will have a greater effect, so in locations where rainfall is more 575 variable within catchments (e.g. Boithias et al. 2014; Terrado et al. 2014), or over timescales where 576 temporal variation becomes an issue, this parameter may become of much greater importance.

577 4.3. LIMITATIONS OF THE MODEL

578 The InVEST NDR model includes only a relatively limited number of the wide range of complex, and 579 spatially and temporally variable processes that influence nutrient transport from land to 580 watercourses (see reviews in Arheimer and Lidén 2000; Edwards and Withers 2008; Parn et al. 581 2012). Whilst this is clearly stated in the InVEST documentation, it is important to explore some of 582 these limitations to remind potential users of the sensible use of the model and to explain the 583 relatively large and variable underestimates of nutrient delivery that our results show. 584 One of the most obvious limitations of applying this model within the UK is that it focuses on diffuse 585 (i.e. non-point) sources of nutrient only, while most UK catchments, especially those in more

populated areas, are also affected by nutrient discharges from WWTWs. This is not a limitation of
the model as such, but it is a problem that needs to be addressed when comparing modelled output
with measured values. This is discussed below under limitations of our validation approach (Section
4.3).

590 A limitation of the model that is harder to compensate for is the presence of catchment specific

591 processes that may affect nutrient transport and export in ways that are hard to predict or capture

592 within model frameworks that are based on an average load per area of land use/land cover class.

593 These include nutrient releases from so-called intermediate sources (because they are neither

594 diffuse nor a predictable point source) such as field drains, septic tanks, farmyard and/or road/track 595 runoff (Edwards and Withers 2008). Such features are difficult to include as a LULC class because 596 they are rarely well mapped and nutrient releases from them are often difficult to predict because of 597 high spatial and temporal variation (Edwards and Withers 2008; Withers et al. 2014). For example, 598 field drains can release large amounts of P into watercourses from agricultural land during storm 599 events, bypassing surface flow and normal retention capabilities (Foster et al. 2003; Heathwaite et 600 al. 2006; Hooda et al. 1999). Such features may be especially important in rural catchments where 601 most other sources are diffuse (Jarvie et al. 2003). In addition, it has been shown that interpolation 602 of infrequent data is unlikely to give reliable estimates of in-stream P loads where temporal changes 603 in stream flow and P concentrations happen very quickly in response to rainfall and surface runoff 604 (Defew et al. 2013).

605 The model can be set to apportion a set amount of nutrient transport to subsurface flow for each 606 LULC class; this is then subject to a simple exponential decay function driven by distance to stream. 607 A value can be defined by the user across all LULC classes (Sharp et al. 2016), but in reality 608 subsurface flow and nutrient retention varies considerably within LULC classes. There are also many 609 features that, whilst contributing to nutrient retention and export, lie below the spatial resolution of 610 most input LULC maps. These include riparian buffer strips or riparian vegetation that can retard or 611 reduce the level of nutrients entering the watercourse (Aguiar Jr et al. 2015; Darch et al. 2015; Lena 612 et al. 1994; Parn et al. 2012). Once nutrient enters a watercourse it may be subject to further 613 retention by aquatic vegetation or uptake by riverine sediments (Jarvie et al. 2005). However, on an 614 annual scale, most of these in stream nutrient sinks are temporary and much of the nutrient 615 delivered to a watercourse from land eventually leaves the catchment in one form or another 616 (Bowes and House 2001).

617 Although the two nutrients are modelled in identical ways by the InVEST model, the extent to which 618 the model is able to reflect the real world flow of the two nutrients is likely to differ, hence our 619 observed differing accuracies for N and P. This is because of differences in anthropogenic sources, 620 temporal and spatial variation is levels of output, and the chemical properties of the two elements 621 and the various forms in which they are usually transported through soil-water systems. One key 622 difference is that N can be removed from the hydrological system by denitrification to atmospheric 623 N₂ and, in some cases, very high retention can be achieved within a watercourse by riverine or 624 wetland vegetation that promotes such processes (Parn et al. 2012; Saunders and Kalff 2001). No 625 equivalent process exists for P (Parn et al. 2012), so at times of high P runoff, the normal retention 626 capacity of any particular land cover class may be more likely to become saturated, leading to higher than expected exports (Koerselman et al. 1990). Phosphorus flows are often dominated by point 627

source releases and temporal factors such as surface runoff during and after storm events. In
contrast, N transport is more often associated with broader land cover patterns, subsurface flow and
soil chemistry (Edwards and Withers 2008; Nedwell et al. 2002; Parn et al. 2012; Withers and Lord
2002).

632 The issues outlined above may be part of the reason why a simple, universally applied reduction of 633 retention coefficients did not substantially improve model accuracy. However, it is also worth noting 634 that the ability of the model to obtain good predictions in terms of the relative magnitude of 635 nutrient export, despite these limitations, suggests that the model and its results are useful if 636 interpreted with caution, especially in order to identify spatial patterns of N or P delivery across 637 catchments or to examine relative change under potential scenarios, which is the intended use for 638 most InVEST models (Sharp et al. 2016). However, the relative export or retention of nutrients alone 639 may not be sufficiently informative for decision makers, who may need to know whether export is 640 sufficient to meet a threshold (e.g. a legal maximum for drinking water or a level known to cause 641 certain ecological impacts) or to place an economic value the service of nutrient retention in terms 642 of avoided water treatment costs. In this case, an understanding of the absolute accuracy of 643 modelled nutrient export figures, and how to best improve this, is key. Of note, the model is open-644 source and its code is regularly updated by the development team or external contributors so that 645 such limitations may be addressed in the future. For example, the NDR model used here was already 646 an improvement over a previous version (Water Quality model, InVEST v3.2).

647 4.4. LIMITATIONS OF THE VALIDATION APPROACH

Validation of the model using the approach detailed in this paper has its limitations. Without actual
measurements of nutrient export to water, estimations of average annual export will always be
subject to a degree of error arising from a variety of factors whatever the method of calculation
used.

652 Firstly, whilst the Beale ratio approach to calculating nutrient has been shown to provide better 653 results than other methods (Dolan et al. 1981; Dunn et al. 2014; Meals et al. 2013; Quilbé et al. 654 2006; Richards and Holloway 1987), it has the potential to underestimate in-stream nutrient load if 655 nutrient sampling does not coincide with periods of peak flow (Quilbé et al. 2006) or peak runoff, as 656 may occur during short duration, extreme weather events. During such events, P transport is very 657 difficult to measure accurately unless sampled at very high frequencies, which is rarely the case for 658 routine monitoring data (Defew et al. 2013). Also, the peak flows recorded by gauging stations may 659 themselves be underestimates where these events affect the accurate measurement of flow (e.g. 660 bypassing of the gauging station by groundwater or flooding, water transfer, etc.). However, our

results suggested that BRE derived values were mostly larger than the modelled N and P values,
even when compared to the interquartile range of BRE values across years or the inter-annual
ranges per catchment, so this is unlikely to be a major driver of this apparent error in model
predictions.

665 Because the model only accounts for nutrients derived from surface runoff, it was necessary to 666 adjust the validation data to estimate the total that would be derived from diffuse sources, only. 667 Using WWTW locations and average per capita nutrient export values is common practice, but 668 potential per capita figures show wide variation between studies, catchments and over time 669 (Edwards and Withers 2008; Johnes 1996; Naden et al. 2016). However, this variation is unlikely to 670 show a systematic bias towards over- or under-estimation across catchments and so our results 671 should provide a fair reflection of model performance in terms of the slope of the linear regression 672 line, even if individual catchments over- or under-estimate the proportion of nutrient export that is 673 derived from point sources. We also quantified the likely extent of this potential error by examining 674 the variation in estimated diffuse source nutrient export imparted by varying the maximum and 675 minimum per capita values for nutrient export from point sources. Even so, there remains a 676 potential for unquantified error in terms of unmapped point sources and variation in per capita 677 values among catchments. Because we excluded catchments where point source nutrient exports 678 appeared to contribute over 50% to the total in-stream nutrient load, we also excluded heavily 679 urbanised catchments. So, our validation cannot inform on the ability of the model to predict diffuse 680 pollution in these types of catchment.

681 4.5. CONCLUSIONS

682 Whilst the InVEST NDR model gives good estimates of the relative magnitude of nutrient exports 683 across catchments, absolute values are frequently underestimated even after calibration of input 684 parameter values. This is to be expected given the simple nature of the InVEST model and the aims 685 of using it to compare the outcomes of change scenarios across a wide range of ecosystem services 686 (Sharp et al. 2015). Key model sensitivities were to nutrient loading and retention factors and the 687 threshold flow accumulation. Input raster resolution had major impacts on model performance only 688 at resolutions coarser than 100m. For resolutions finer than this, there was little in the way of 689 increased accuracy to offset the increased model run time and output data volume.

690 Collating the data sources for input and validation of the model, even in such a well-studied region 691 such as the UK, was time consuming and complex. Similar difficulties are likely to be encountered in 692 regions that have less frequent monitoring schemes for nutrients and water flow. Since one of the 693 stated aims of the InVEST model is to allow meaningful analyses to take place in data-poor regions,

- 694 we recommend the following uncertainty assessment analyses: exploration of alternative input
- datasets for the study region, sensitivity analyses on loads and retention efficiencies for dominant
- 696 LULC types, TFA, and k_b , and a thorough exploration of the model outputs before using them to
- 697 inform decisions. This reflects the recommendations of the designers of the InVEST NDR model
- 698 (Hamel et al. 2015; Sharp et al. 2016) and the findings of previous studies across a number of
- 699 ecosystem services (Boithias et al. 2014; Pessacg et al. 2015; Redhead et al. 2016; Sánchez-Canales
- 700 et al. 2012).

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