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Development of a Chemical Source Apportionment Decision Support Framework for Catchment Management

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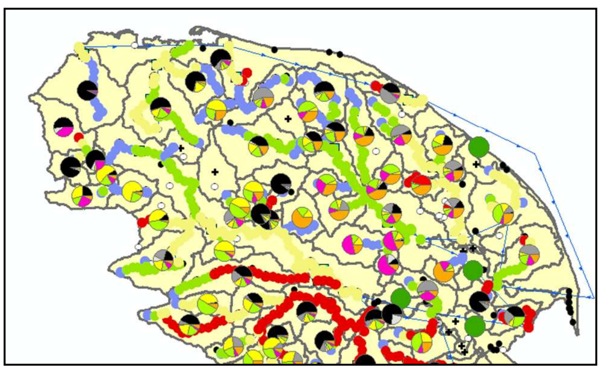
Research Article – Environmental Modeling

Abstract Art



Key words

Chemical, source apportionment, nutrients, metals, environmental modeling

Abstract

EU legislation, including the Water Framework Directive, has led to the application of increasingly stringent quality standards for a wide range of chemical contaminants in surface waters. This has raised the question of how to determine and to quantify the sources of such substances so that measures can be taken to address breaches of these quality standards using the polluter pays principle. Contaminants enter surface waters via a number of diffuse and point sources. Decision support tools are required to assess the relative magnitudes of these sources and to estimate the impacts of any programmes of measures. This paper describes the development and testing of a modeling framework, the Source Apportionment Geographical Information System

(SAGIS). The model uses readily available national data sets to estimate contributions of a number of nutrients (nitrogen and phosphorus), metals (copper, zinc, cadmium, lead, mercury and nickel) and organic chemicals (a phthalate and a number of polynuclear aromatic hydrocarbons) from multiple sector sources. Such a tool has not been available on a national scale previously for such a wide range of chemicals. It is intended to provide a common platform to assist stakeholders in future catchment management.

Introduction

The European Union Water Framework Directive (WFD)[1] sets criteria for water bodies to meet a defined status categorised as ‘good’, which requires chemical standards for 33 priority and priority hazardous substances and groups of substances to be achieved, in addition to standards for ecology, hydrology and hydromorphology. The Environmental Quality Standards (EQSs) set for these substances are generally more stringent than existing EQSs that were under other previous Directives, including the Dangerous Substances Directive.[2]

Historically, the principal method for improving river water quality has been to place restrictive discharge consents on point source discharges, including those from wastewater treatment works. In the UK, a combination of the development of a less polluting industrial base as a response to more stringent regulation in the form of EU Directives and downward pressure on limit values from other point sources, means that for a number of substances, diffuse sources from agriculture, urban runoff, soil erosion and discharges from abandoned mines make an increasingly important contribution to exceedances of EQSs.[3] The WFD advocates the application of the ‘polluter pays principle’[1] to ensure that any one sector is not unduly burdened with the requirement to reduce discharges to meet an EQS. To plan to meet the stringent standards set by the Directive it is therefore necessary to quantify the significance of all sources to an EQS exceedance in any given water catchment. In many instances it is likely that mitigation measures targeting multiple sources / sectors will be needed to achieve good ecological status, so a clear appreciation of relative contributions is essential.

In order to establish plans to comply with new EQSs it is necessary for regulators and regulated alike to have tools to test and support planning decisions. A number of models have been developed to predict inputs of chemicals from agricultural diffuse sources; notable amongst these in the UK are PSYCHIC for soil and phosphorus and NEAP-N for nitrogen. NEAP-N is a simple model created by ADAS that looks at leachate from different land uses.[4] It incorporates details down to for example a livestock or fertilizer management level. Output is a visual representation of grid squares over the catchment of interest, representing predicted change in concentrations per hectare. The model does not include a within stream fate component, so it is primarily used as a source of information on agricultural inputs of nitrogen into a catchment based water quality model. PSYCHIC, The Phosphorus and Sediment Yield CHaracterisation In Catchments model has been developed by ADAS, NSRI, CEH-Wallingford, and the Universities of Exeter, Reading and Sheffield through a Defra funded research programme.[5] PSYCHIC was developed to model phosphorus (P) and sediment transfers in agricultural systems to investigate options to reduce P delivery from land to rivers, particularly through identification of hotspots and an associated field-scale risk assessment exercise.

Once discharged to a watercourse, any given chemical will be subject to dilution and undergo various biogeochemical processes that might be incorporated into a model. Water Quality models include the United States Environmental Protection Agency (USEPA) model QUAL2E;[6] the MIKE series of models that is developed by the Danish Hydraulics Institute, and the Systeme Hydrologique European (SHE)[7]; The most used models by the Environment Agency of England and Wales are SIMCAT and TOMCAT. SIMCAT is able to simulate a statistical distribution of discharge and water quality data for multiple effluent inputs within a catchment. It is capable of simulating up to 2500 random boundary conditions (also known as the Monte Carlo approach), based on the input data, SIMCAT produces a distribution of results from which an assessment of the impact can be made on the predicted mean and ninety-five percentile concentrations.[9] SIMCAT allows for inputting decay constants based on a first order decay rate and provides options for point and diffuse source inputs. In addition the SIMCAT source code is sufficiently flexible to allow upgrades to include such options as inputting partition coefficients to allow concentrations of, for example, metals, to be split into dissolved and particulate bound concentrations.

Regulators have also sought to develop screening models for assessing pollutant pressure in order to plan relevant measures on a national scale. The Scottish Environmental Protection Agency (SEPA) have developed such a screening tool; the Diffuse Pollution Screening Tool (DPST)[10] which has drawn together large national datasets for a number of different types of chemicals including metals, nutrients, pesticides and sanitary determinands (BOD, ammonia). However, the focus of the model is on source apportionment alone, rather than predicting in-river concentrations, partly owing to the fact that there is no national water quality model for Scotland, akin to that of SIMCAT for England and Wales.

The difference between source apportionment and water quality prediction is a key distinction. Source apportionment models have value in risk assessment of determining input loads and to some degree locations, but their application to water quality modeling is not straightforward. Modeling of the mixing of inputs, taking account of the variability of flow and load and incorporating appropriate processes of chemical behaviour add a considerable level of complexity. There are currently few models which can do this on a local or regional scale and none on a national scale. One model developed to achieve catchment management of a regional scale is the GREAT-ER model (Geographically-referenced Regional Exposure Assessment Tool for European Rivers). The model was originally developed to assess the exposure risk of new substances discharged to sewer from predominantly domestic sources, but has been expanded to include diffuse and point sources within a number of German catchments. GREAT-ER is a hybrid Monte-Carlo deterministic model which allows a user to calculate the predicted environmental concentration (PEC) for a substance, taking into account its geographical and temporal distribution, to produce a statistical output and perform 'what-if' scenarios Data entry and selection is via a GIS interface and In the receiving watercourse, chemical processes are represented by conservative dilution, first order decay (similar to SIMCAT) or more complex processes (similar to QUAL2E). Output is provided as annual statistics produced longitudinally downstream and converted into PEC values, which are displayed via the GIS interface. The modeling system is open-source (http://www.great-er.org/pages/home.cfm) with the aim of creating a live development framework. The GREAT-ER model has been recently applied to the Ruhr catchment for the source apportionment of zinc which includes background inputs, discharges from mining activities, runoff, sewage treatment plant sources and diffuse agricultural contributions.[11]

The development of river basin management plans to meet WFD objectives requires the assessment of a synthesis of local and national, ppoint and diffuse source measures, this paper describes a modeling framework developed to utilise for the first time, national datasets for multiple parameters including hydrology, rainfall, modelled discharges of chemicals, reported discharge loads, and spatial datasets including the locations of wastewater treatment works and smaller on-site works often septic tanks, combined sewer overflow locations, output from diffuse pollution risk models, road and river system networks combined within a GIS based modeling framework to provide estimates of pollutant loads and in-river concentrations of chemicals at water body scale for the whole of England and Wales.

Methods

The Source Apportionment-GIS (SAGIS) modeling framework integrates information from multiple sources. Loads from different source sectors are derived from coefficients expressed as an annual or monthly mean load with corresponding standard deviation. Point sources are represented as mean and standard deviations of concentrations and flow with the option of breaking down inputs into monthly values to allow simulation of seasonal effects. Diffuse sources are represented as mass per year, or month, per km^2. All loads are routed into associated river reaches using one of 18 regional SIMCAT models covering England and Wales. Simcat models are being developed for Scotland and so currently only loads can be derived. To cover the whole of Great Britain (England, Wales and Scotland) on this basis, the use of datasets with national coverage was imperative to provide both consistency of approach and the ability to manage and update data. A common map projection was used for all databases and mapping based on a $1km^2$ grid of England, Wales and Scotland. Such GIS mapping calibration and validation had previously been undertaken as part of previous projects associated with the hydrological and diffuse source components. Detailed information regarding the methodologies used to calculate loads for each source is provided elsewhere.[12] However, a brief description of the data and method used to derived load estimates is provided in the following section.

Table 1 summarises the type of source (both diffuse and point) and notes whether loads to surface waterbodies were either derived via an established model or were calculated as part of this research. Figure 1 provides a schematic for the structure and key components of the SAGIS decision support framework.

Table 1 Summary of methodology used to calculate loads discharged to waterbodies

Category	Source	Metals	Nutrients	Organics
Agriculture – Arable and Livestock	Diffuse	n/a[1]	PSYCHIC (P), NEAP-N models	n/a
Highway (non urban runoff)	Diffuse	Highway Agency HAWRAT model	Highway Agency HAWRAT model	Highway Agency HAWRAT model
Urban runoff	Diffuse	Calculated	Calculated	Calculated
Background erosion	Diffuse	PSYCHIC model + calculated	n/a	PSYCHIC model + calculated
Onsite wastewater treatment systems	Diffuse	Environment Agency model[2] + calculated	Calculated	Calculated
Atmospheric deposition	Diffuse	Calculated	P n/a N within NEAP-N models	Calculated
Treated wastewater effluent	Point	Measured[3] and defaults	Measured and defaults	Measured and defaults
Storm tanks/combined sewer overflows	Point	Calculated	Calculated	Calculated
Industrial discharges	Point	Environment Agency Measured/reported	Measured/reported	Measured/reported
Mine water discharges	Point	Environment Agency Measured/reported	n/a	n/a

[1] Included in erosion category; [2] EA model used to predict locations of onsite wastewater treatment systems
[3] based on EA and Water Company data (flow and concentration);

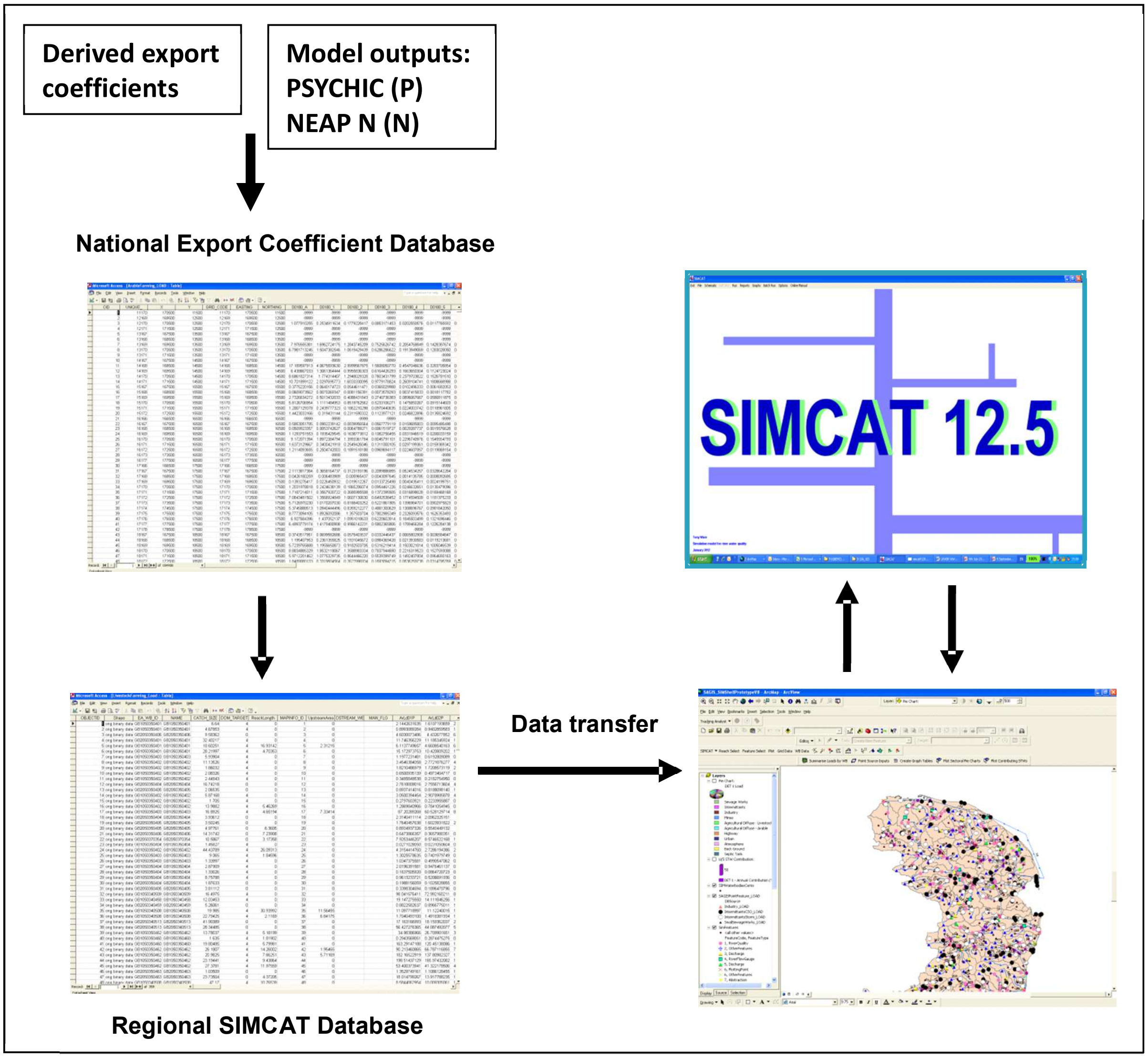


Figure 1 Schematic diagram for SAGIS tool structure

Tables which list the key datasets used to derive the exported loads from each source and information as to how the datasets were used to derive the calculated loads to waterbodies are provided in Table 1 and 2 of the Supporting Information respectively.

Owing to WwTW inputs being significant for many substances of interest, it was critical to utilise as much monitoring data as possible to derive accurate loads entering receiving waters. In the absence of effluent data for WwTW, ie for WwTW where there is not a requirement to determine the chemicals of interest in their effluent owing to the absence of a consent, then default values were required. All available concentration data were collected and collated for Environment Agency monitoring between 2007 and 2009 inclusive, which added up to a maximum of over 2,000 results for phosphorus and nitrogen, several hundred for the metals to very few for the organic determinands. In most cases a mean concentration was chosen as the default value. For phosphorus because the non-consented works without effluent data would not have had phosphorus reduction measures installed, a default value was generated from all monitoring data reported above 2 mg-P/l. Details of the monitoring data used and the default values chosen are provided in Table 3 of the Supporting Information.

Inputs to SIMCAT for point sources also require a flow for WwTW effluent discharges in order to generate a load.

Flows for the works were based on a number of collated data in the following hierarchy of available data:

1) Measured flows and standard deviations provided by the water companies
2) Consented DWF
3) Populations multiplied by an average flow per capita per day (from all sources) assumed to be 250 l/capita/day.

A summary of the number of WwTW applicable to each category is provided in Table 4 of the Supporting Information.

Reported literature runoff data[15] was used to generate concentrations of the substances of interest in road runoff expressed as an event mean concentration (which takes account of the 'first flush' effect and subsequent reduction in concentration with increasing rainfall) and in domestic dry weather flow (Table 2).

Table 2 Runoff and dry weather flow concentration data[13]

Concentrations used	Event Mean Concentration for Road Runoff (µg/l)	Domestic raw sewage (µg/l)
Copper	34.7	186.1
Zinc	82.5	62.6
Total PAHs	0.68	0.76
Fluoranthene	0.06	0.093
Naphthalene	0.08	0.077
Benzo(a)pyrene	0.03	0.025
Benzo(b)fluoranthene	0.03	0.030
Benzo(k)fluoranthene	0.04	0.030
Benzo(ghi)pyrene	0.03	0.025
Indeno(123-cd)pyrene	0.03	0.025
DEHP	20	33.1
Total Nitrogen (mg/l)	1.93	39.7
Total Phosphorus (mg/l)	0.27	13.9

Water quality monitoring data provided by the Environment Agency and SEPA was used for model testing purposes.

Each source was represented within a Microsoft Access™ database either as a point source with an X and Y,UK national grid location coordinate or as an individual 1 km^2 grid (approximately 150,000 for England and Wales) (Figure 1). The main database is then split into 18 regional Access databases (see Figure 1 in the Supporting Information) which form the attribute tables behind the features in ArcMAP 9.3™ GIS software. The functionality with ArcMap and bespoke macros developed in Visual Basic are then used to extract the necessary data and generate the text file required to run SIMCAT, a stochastic water quality model. SIMCAT can be run from within SAGIS and provide outputs (total and dissolved concentrations and loads for metals, total concentrations and loads for nutrients and organics) which are fed back into ArcGIS to provide cartographic, graphical and spreadsheet outputs (Figures 2 and 3).

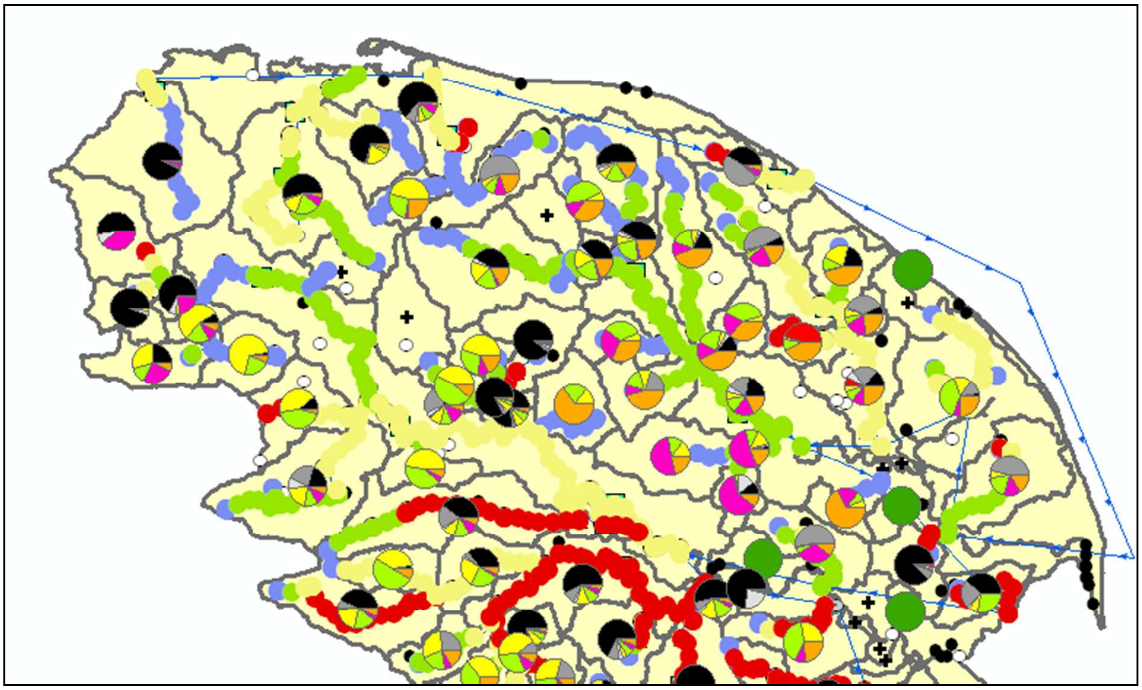


Figure 2 Example source apportionment from SAGIS for phosphorus in East Anglia

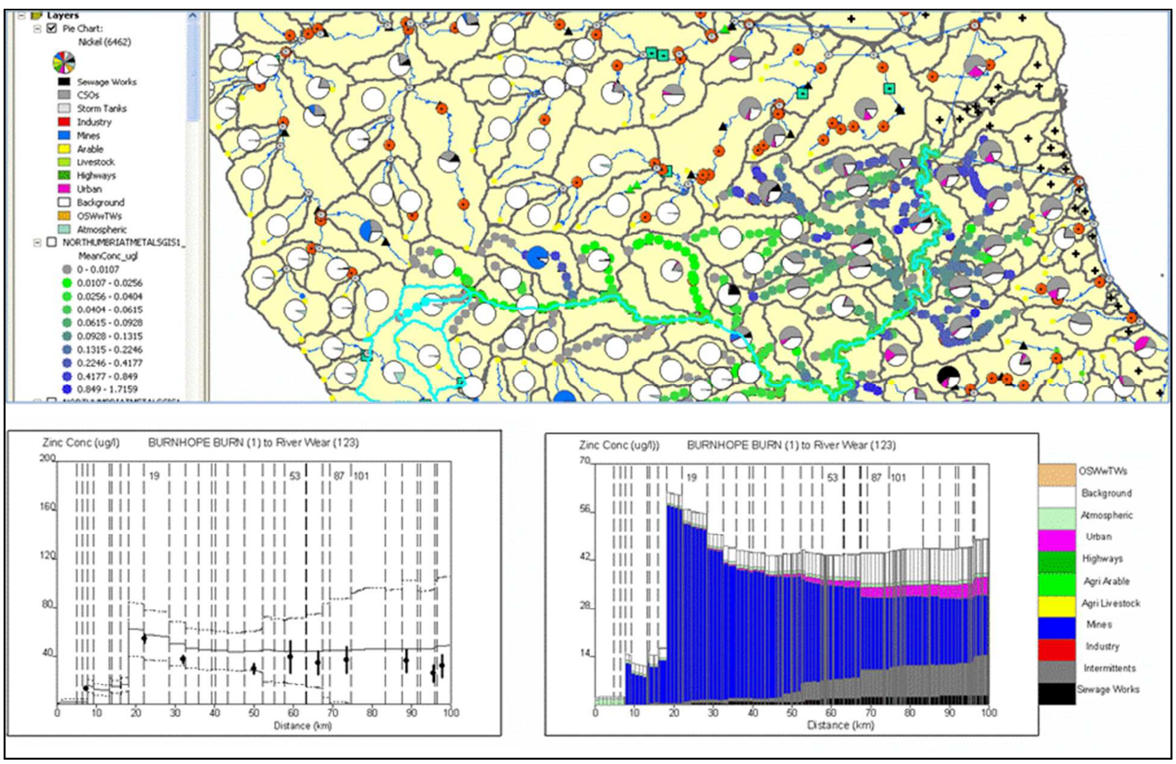


Figure 3 Example outputs from SAGIS

Results

The model was initially populated with input data for total nitrogen, total phosphorus, total copper, zinc, nickel, lead, cadmium and lead, PAHs (naphthalaene, anthracene, fluoranthene, benzo-a-pyrene, benzo-b-fluoranthere, benzo-k-fluoranthene, benzo-ghi-perylene, indeno-123,cd-pyrene) and diethylhexylphthalate. Extension to other substances is under ongoing consideration.

The SAGIS model provides a number of outputs (Figures 2 and 3), including:

- Colour coded concentrations within the river system at 1km intervals which can be aligned with compliance assessment guidelines (e.g. EQS or ecological status under the WFD)
- Pie charts illustrating the relative contributions from all upstream sources to the load or concentration at the outflow from each waterbody (approximately 7,000 in England and Wales)
- Pie charts illustrating the relative contributions from different sources to the load on a waterbody basis
- Cumulative concentration from each source along a river length defined by the user
- Predicted versus observed concentrations where monitoring data is available

The ability to graphically present the percentage contribution from the different point and diffuse source sectors provides a very visual representation of the main contributors to loads or concentrations of a chemical to any given waterbody. Such outputs are vital in engaging stakeholders in the process of improving water quality under the Water Framework Directive.

When integrating models from many sources for different components of physic-chemical environments, with varying spatial and temporal specificity, the question of parameter estimation (i.e. accuracy of export coefficients) and potential error propagation becomes paramount. To test the predictive skill of SAGIS based on the National / default data layers a comparison between predicted and measured concentration data was undertaken for three selected catchments of differing typology (mine dominated – river Wear in the NE of England, part of the Northumbrian model and mixed, urban – river Tame Midlands, part of the river Trent model and rural river Avon part of the SW England model) (see Figure 2 in the Supporting Information).

The process aimed to:

- Identify any data transfer errors in the development of the export coefficient databases and the input of these to SIMCAT
- Identify where the default export coefficients based on national datasets do not provide a good representation in individual catchments and may require modification; either to the methodologies, the associated assumptions or the underlying data
- To test the accuracy of the default partition coefficients in predicting dissolved metal concentrations.
- Identify any underlying uncertainties that may affect the performance in the model
- Identify key improvements that might be made to the tool to improve the predictive capability of the model at the National and catchment scale.

The SAGIS model has been developed for use at a waterbody and catchment spatial scale and consequently has utilised nationally derived default assumptions where measured data is not available, Finer resolution may be possible, but the accuracy of outputs would need to be tested at a local level, potentially requiring more detailed local data.

There are two key components of the model, the loads discharged to rivers, waterbodies and catchments and their conversion into concentrations using the SIMCAT water quality model. Although it would have been desirable to compare measured and predicted loads entering the aquatic environment, there are no national databases for measured loads for nay of the chemical parameters or input sectors. There is however, an extensive national water quality monitoring database held by the Environment Agency which was used for the purpose of testing the SAGIS model. Furthermore, compliance testing is based on measurement of concentrations against an EQS, and so it is vital that any model used by stakeholders provides concentration data so that the impacts of any future measures applied to improve water quality can be measured against EQS compliance.

Figures 4 and 5 provide summary statistics for the output of the SAGIS tool compared with observed data (means derived from all monitoring between 2007 and 2009 inclusive) for each of the three regional model areas for metals and nutrients respectively.

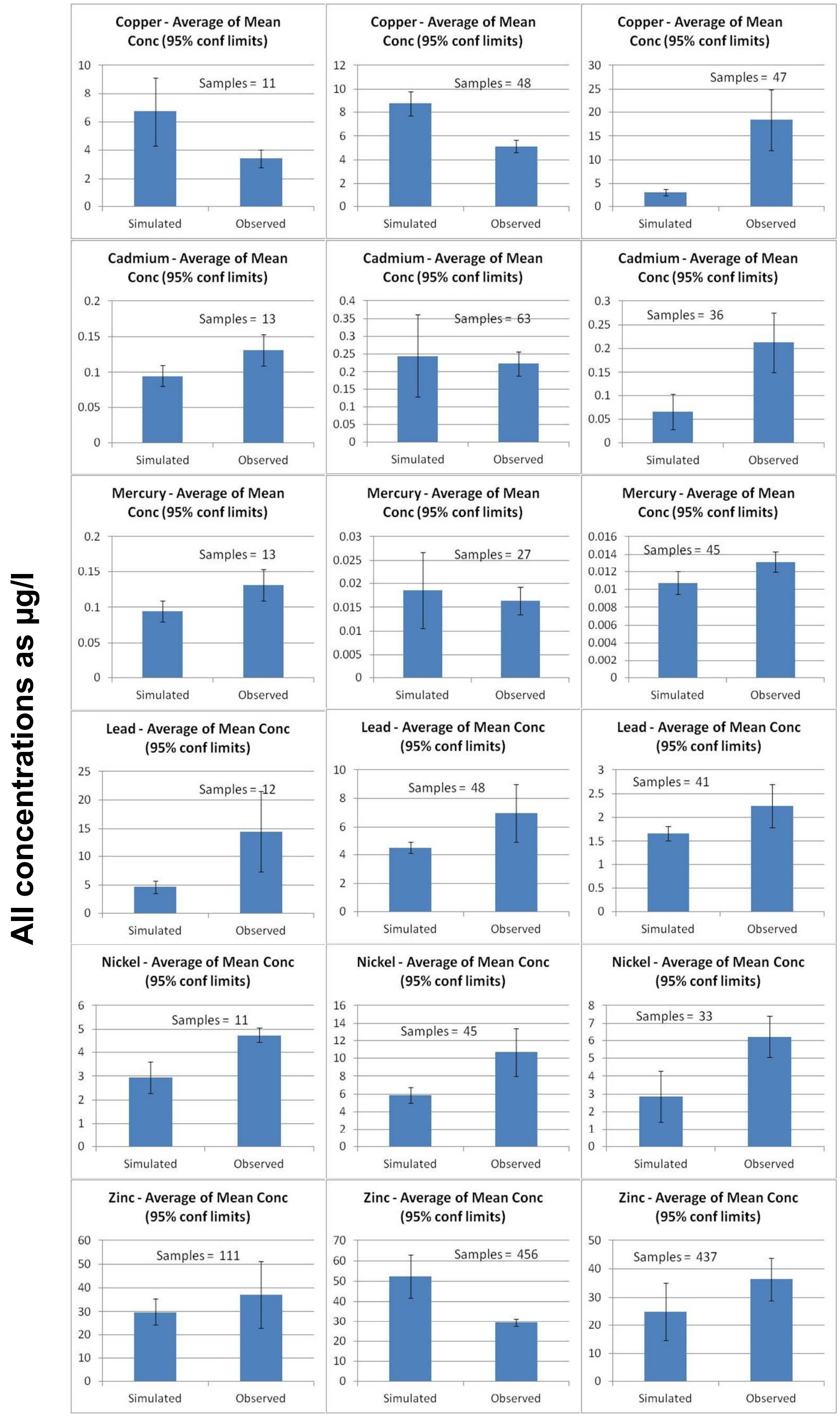


Figure 4 **Comparison between observed and simulated concentrations for all data generated from the three regional models for metals**

The data in Figure 4 provide averages and 95% confidence intervals for a number of metals for which concentrations can be simulated within the SAGIS programme. For copper all predictions are of the same order, although simulations in the Northumbria and Trent model tend to overestimate levels in the catchment slightly, with the reverse for the SW model. It should be noted that for the SW model, observed values were biased towards a number of highly mineralised sites in the west of the catchment explaining the lower predicted value. Cadmium simulations were comparable for Northumbrian and Trent regions but similar to copper, the model underpredicted concentrations in the SW, for the same reasons. Mercury, being un-influenced by UK mineralogy, shows good comparability between predicted and observed means, although it should be noted that mercury monitoring data is somewhat limited owing to many reported concentrations being less than limit of detection. Lead concentrations, too are generally comparable, although in this case, the NE mineralogy is dominated by lead/zinc mines and so as for Cu/Cd in the SW, the model underpredicts lead inputs from this region. Concentrations in the Trent and SW model are comparable and low. For nickel a metal for which anthropogenic inputs dominate sources, a good comparison between measured and predicted means is observed. Finally, for zinc, levels are relatively high and variable owing to both the ubiquitous nature of zinc and its presence in soil, minerals and anthropogenic discharges. However, the comparability is still good even for the mine dominated sites in the Northumbrian model.

Overall it is clear from Figure 4 that given the nature of the generic datasets used within the SAGIS model, comparisons with observed data may be considered very good. Under estimates compared with measured data are associated with mineral-rich areas where although some point source loads are accounted for, ie major adits which are monitored for flow and concentration, thus providing a load, there are many diffuse inputs not accounted for from minor adits, leaching and soil loss from spoil tips and old processing sites. Previous studies in the Tamar catchment, for example, have highlighted the loads of metals that can potentially arise from diffuse sources, which may match or even exceed point source inputs.[16] The model is currently being updated to take account of diffuse mine inputs.

Data for nutrients (Figure 5) shows excellent agreement between predicted and observed values for phosphorus and nitrate with significantly high levels in the urban

Trent region associated with discharges from wastewater treatment works (WwTW). Both of these inputs are dominated by a combination of agricultural diffuse and WwTW inputs. Given that agricultural inputs are derived from well developed and tested models and WwTW inputs are derived from extensive monitoring data, it is unsurprising that comparability is good. Furthermore, it needs to be noted that although observed data are collected all year round, sampling cannot take place during periods of heavy rain or flooding for safety and practicality reasons. Consequently, significant loads entering the waterbodies during high rainfall events particularly substances associated with particulate matter may be underestimated via routine monitoring data, thus leading to an underestimation compared with predicted data.

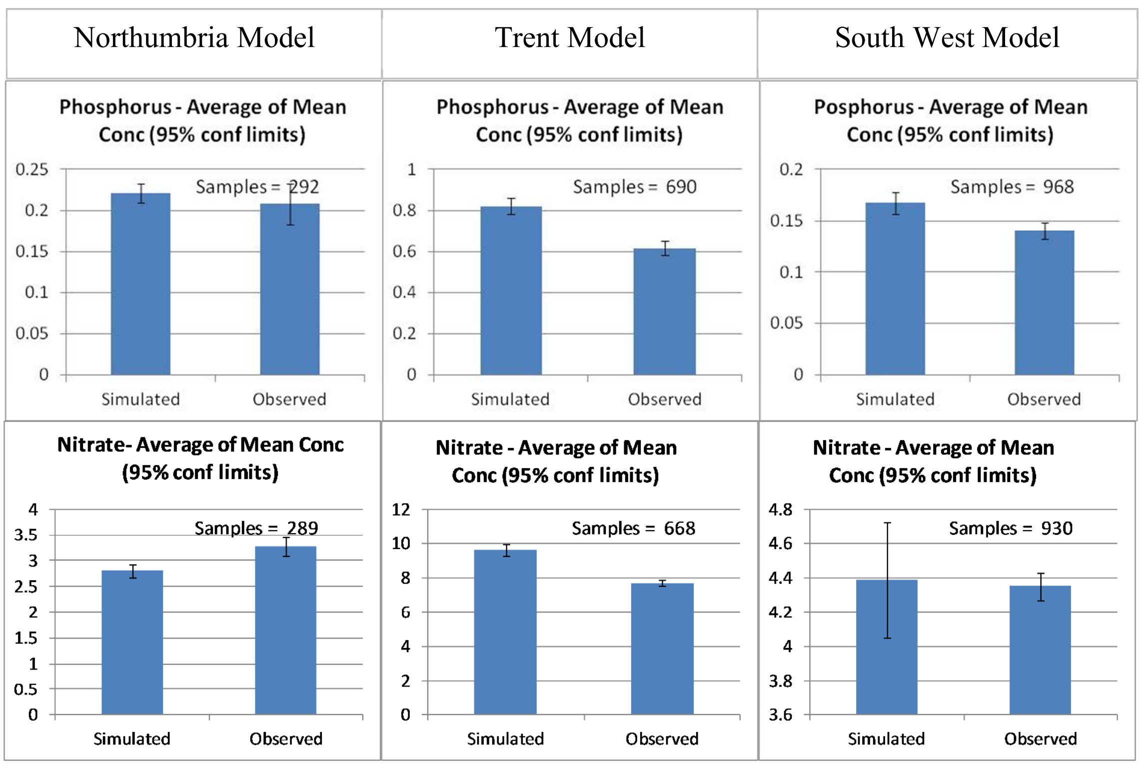


Figure 5 **Comparison between observed and simulated concentrations for all data generated from the three regional models for nutrients**

Although in some cases there appears to be a degree of statistically significant bias they don't indicate a bias that is likely to be important in terms of status assessment or catchment management. This suggests that either estimates of variance in the model are too low or that there is bias in monitoring; or both.

The model was further validated by comparing measured versus predicted concentrations within the individual rivers (Wear, Avon and Tame). Examples of simulated concentrations of the case study substances in the main river channel are provided in the Supporting Information (Figures 3, 4 and 5). There was insufficient observed information for the organic substances to allow a meaningful comparison between observed data and model output. For the river Wear in Northumbria zinc inputs are dominated in the upper catchment by a limited number of mine water inputs from abandoned zinc/lead mines. The model predicts accurately the step change in concentration 25 km downstream of the source as major mine inputs enter the river. After a small amount of dilution, levels then remain at ~ 32 μg/l to the tidal limit. Comparison between predicted and measured values is excellent and further supports the validity of the model outputs generated from summing a variety of point and diffuse loads entering the river. Zinc levels in the river Tame are high owing to inputs from historically contaminated land and resulting leachates (thought to be an historic landfill site, EA data). Concentrations of several 100 μg/l are measured in the upper catchment. These are not accurately predicted because no loads for inputs from landfill or other contaminated land (with the exception of large mine sites) were available on a nationwide basis. Further downstream, however, after substantial dilution and where levels are influenced mainly from sewage effluent discharges (for which adequate datasets are available), predictions match observed values. For the agricultural catchment of the River Wylye, levels of zinc are substantially lower and predictions mostly lie within the 95% confidence intervals of measured data.

A similar exercise was carried out for phosphorus (Supporting Information, Figure 4). The river Wear is subject to inputs from upland low intensity livestock farming and low population centres. Overall predicted concentrations track observed values from low concentrations of phosphorus in the upper catchment, slowly rising downstream as larger towns provide phosphorus inputs to the river via sewage works. In all cases except one anomalously high observed concentration predicted values were slightly in excess of measured values, potentially owing to the PSYCHIC model over estimating agricultural loads or a slight bias in the relationship between loads and river flow used in the model. In a catchment such as the Tame, where accurate data for the main inputs (sewage effluents) are available, predictions versus observed values matched consistently down the catchment. A similar situation occurred for phosphorus in the Wylye/Avon, a predominantly chalk catchment dominated by arable farming, with good agreement between measured and predicted values throughout the river length. Observed and predicted concentrations of phosphorus show an increase at the 11km mark owing to a sewage treatment works input and remain relatively consistent thereafter..

Simulated and observed nitrate concentration in the river Wear showed excellent comparability with a gradual increase down the catchment as the contribution from sewage effluents slowly increases. A similarly close agreement was observed for the Tame, although much higher concentrations were observed and simulated (ca. 10 mg-N/l) owing to it being a sewage effluent-dominated catchment. The Wylye being a more rural catchment exhibits lower concentrations which again are influenced by an effluent discharge 11 km downstream of the source.

Overall, given the acceptable level of comparability between measured and predicted concentrations it can be concluded that the model may be used for river planning purposes with confidence, particularly when considering the impacts of applying certain programmes of measures to meet environmental quality standards. This will be of particular importance given mean catchment concentrations for Cd, Pb and Hg will exceed the WFD EQS at certain sites with the potential of P, Zn and Cu also exceeding UK derived limits in certain waterbodies. Cases where there is a statistically significant bias between simulated and predicted data may require further investigation at a local scale which is something regional Environment Agency staff have been recommended to undertake.

Discussion

For the first time a model has be developed at a national scale which combines predictions of input loads for all major sources of a contaminant with a water quality model to predict in-stream concentrations for a number of determinands including organics, metals and nutrients. Previously reported source apportionment models have been developed at a catchment scale for single chemicals such as zinc[11] but none has used national datasets to provide predictions over an area of approximately 150,000 Km^2 and including over 100 river catchments.

It is anticipated the framework could be used for:

- Water quality planning. SIMCAT has been widely used for water quality planning and setting of wastewater consents. All of the existing functionality of SIMCAT is retained in the tool and the diffuse and point source sector inputs can be ‘switched off’ and the model used in the normal way if required. By using the tool to estimate the contribution of the various diffuse and point sources, this traditional use of SIMCAT can be enhanced by providing a better indication on the sources of chemicals to improve planning of measures.
- Source control. SAGIS provides national and regional scale information on source apportionment which can be used to inform national policy on source control. For example, for organic chemicals the SAGIS could be used to indicate whether the main sources of chemicals are from controllable sources (e.g. rather than background).
- Reporting. SAGIS provides a range of visualisation options for chemical inputs and predicted within-stream concentrations loads which could be readily used for reporting of pressure characterisation and compliance for River Basin Management plans.
- Testing of measures. SAGIS provides a framework to test the effectiveness of measures related to each source sector and these can compared using the model output and visualisation tools.
- Catchment management stakeholder engagement. SAGIS provides an overview of the contribution of all sources of chemicals and, therefore, provides the ‘big picture’ for a catchment to identify the dominant sectors and sources and highlight where additional information is required or measures should be targeted. Presentation of this overview using the visualisation functionality with SAGIS provides a valuable starting point for stakeholder engagement through provide the context at the catchment scale.
- Identify further monitoring and research. By bringing together a wide range of national datasets, key areas of uncertainty in estimation of source apportionment have become clearer which could provide a focus for improving source data or the methodologies to create the export coefficient databases. By showing which sectors are likely to be important for each chemical, the tool provides a focus for where additional research and data collection would be beneficial. Without this overview, this effort might be misdirected.

It is important to understand that the current version of the SAGIS is based on national datasets and so lacks refinement at a local level. It is estimated that for catchments in excess of 50 km^2 confidence in the model outputs can be considered good. The model provides an open framework derived from the best available national data and knowledge which may easily be refined at a local level.

No calibration or model conditioning has been carried out on the tool at present and default values have been used in many cases; for example travel times and decay rates. For assessment of compliance with water quality standards, data refinement, calibration of decay rates and travel times (using the approach traditionally adopted for SIMCAT) or conditioning of the export coefficients need to be carried out or the assessment should take into account the difference between model output and observed data.

The next step of its development is to provide it to local Environment Agency staff to input data considered to be better than current default data currently in the databases. Furthermore, additional substances are to be added over the coming years and the databases maintained to ensure they are up to date. There will be a particular focus on phosphorus in the next sets of river basin plans under the WFD and so the interaction and data generated by PSYCHIC and used by SAGIS will be more closely examined in the next phase of development, along with increasing the coverage of the model from rivers to lakes, estuaries and coastal waters.

The SAGIS model represents the first comprehensive source apportionment tool to be developed on a national scale for such a wide variety of chemicals. To meet ever more stringent standards multiple interventions will be required to reduce discharges from point and diffuse sources. SAGIS will assist regulators in making effective decisions regarding how best to meet challenging water quality targets by identifying the predominant source of a chemical. It also allows practitioners from sectors such as the water industry to plan future improvements within a catchment at wastewater treatment works where the greatest benefits on receiving water quality will be achieved. This is of particular importance for ubiquitous substances such as nutrients and metals where the impact of different sources can vary throughout a catchment.

SAGIS has been shown to provide accurate predictions of in-river concentrations for metals and nutrients at a catchment scale, providing a degree of confidence in the predicted outputs. The Environment Agency of England and Wales in conjunction with key stakeholders will be using and developing the model as part of the second cycle of river basin planning from 2013 onwards.

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Supporting Information

Tables of databases, default values and information used to develop the model are provided in the supporting information in addition to comparison data for model outputs versus observed data.

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