09 – UNDERSTANDING HYDROLOGICAL FLOW PATHS IN CONCEPTUAL CATCHMENT MODELS TO IMPROVE WATER QUALITY MODELLING

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Abstract

Increasing pressures on water quality due to intensification of agriculture have increased the need for environmental modelling to accurately simulate the movement of diffuse (nonpoint) nutrients in catchments. As hydrological flows drive the movement and attenuation of nutrients, individual hydrological processes in models should be adequately represented for water quality simulations to be meaningful. In particular, the relative contribution of groundwater and surface runoff to rivers is of interest, as, for example, higher nitrate concentrations in surface waters are strongly linked to catchments with proportionately larger groundwater contributions to the river.

In this study, uncertainty analysis was used to investigate parameter sensitivities and flow partitioning of three conceptual hydrological models simulating 31 Irish catchments. We compared two established conceptual hydrological models (NAM and SMARG) and a new model (SMART), produced especially for water quality modelling. In addition to the criteria that assess streamflow simulations, a ratio of average groundwater contribution to total streamflow was calculated for all simulations over the 16 year study period. As measured time-series of groundwater contributions to streamflow are not available at catchment scale, the groundwater ratios were evaluated against average annual indices of base flow (from the OPW) and estimates of deep groundwater flow (from the Geological Survey of Ireland) for each catchment. The exploration of sensitivities of internal flow path partitioning was a specific focus to assist in evaluating model performances. Results highlight that model structure has a strong impact on simulated groundwater flow path contributions. Sensitivities to the internal pathways in the models are not reflected in the usual (flood forecasting) performance criteria results. This demonstrates that simulated groundwater contribution should be constrained by independent data to ensure results within realistic bounds if such models are to be used in the broader environmental sustainability decision making context.

1 INTRODUCTION

Catchment-scale modelling is used to understand complex interactions between anthropogenic activities, climate and hydrological processes. Recent modelling studies in Irish catchments have simulated a range of contaminants, such as, faecal bacteria indicators (Coffey et al., 2010, Bedri et al., 2014), cryptosporidium (Tang et al., 2011), sediment yields (Rymszewicz et al., 2015) and nutrient losses (Jennings et al., 2009, Greene et al., 2011, Nasr and Bruen, 2013). Investigating nutrients in Irish catchments is of particular interest as environmental objectives from the Water

Framework Directive (2000/60/EC) and Nitrates Directive (91/676/EEC), compete with increasing demand for clean water for drinking and food production.

As water mobilises and transports solutes through the landscape, water quality models are often coupled with hydrological modelling in order to capture solute dynamics during rainfall runoff events. Therefore the relevant hydrological processes in models such as MIKE (DHI, 2013) and GWLF (Schneiderman et al., 2002) should be adequately represented in order for water quality simulations to be meaningful (Medici et al., 2012). There is a growing body of literature investigating hydrological model structure uncertainty (Wagener et al., 2001, Clark et al., 2008, Kavetski and Fenicia, 2011, Gupta et al., 2012). Focus is increasingly turning to the internal movement of water within these conceptual models to investigate if each of the simulated processes contributing to the total flows are realistic (e.g. Kokkonen and Jakeman, 2001, Fenicia et al., 2011). This hydrological partitioning is particularly important when coupling flow simulations with water quality, as the flow paths, each with different travel times and passing through different strata, can have significant effects on solute transport and attenuation (Futter et al., 2014).

The aim of this study was to compare the suitability of hydrological model representation of the internal flow paths in Irish catchments. We assessed a new model that we developed with a focus on sub-surface flow paths, SMART, along with two well-established conceptual models, NAM and SMARG. The groundwater and surface water interactions simulated by the internal flow paths of the three models are compared using Monte Carlo simulations. The analysis is carried out on multiple goodness-of-fit metrics with the three models simulating a 16 year period in 31 Irish catchments.

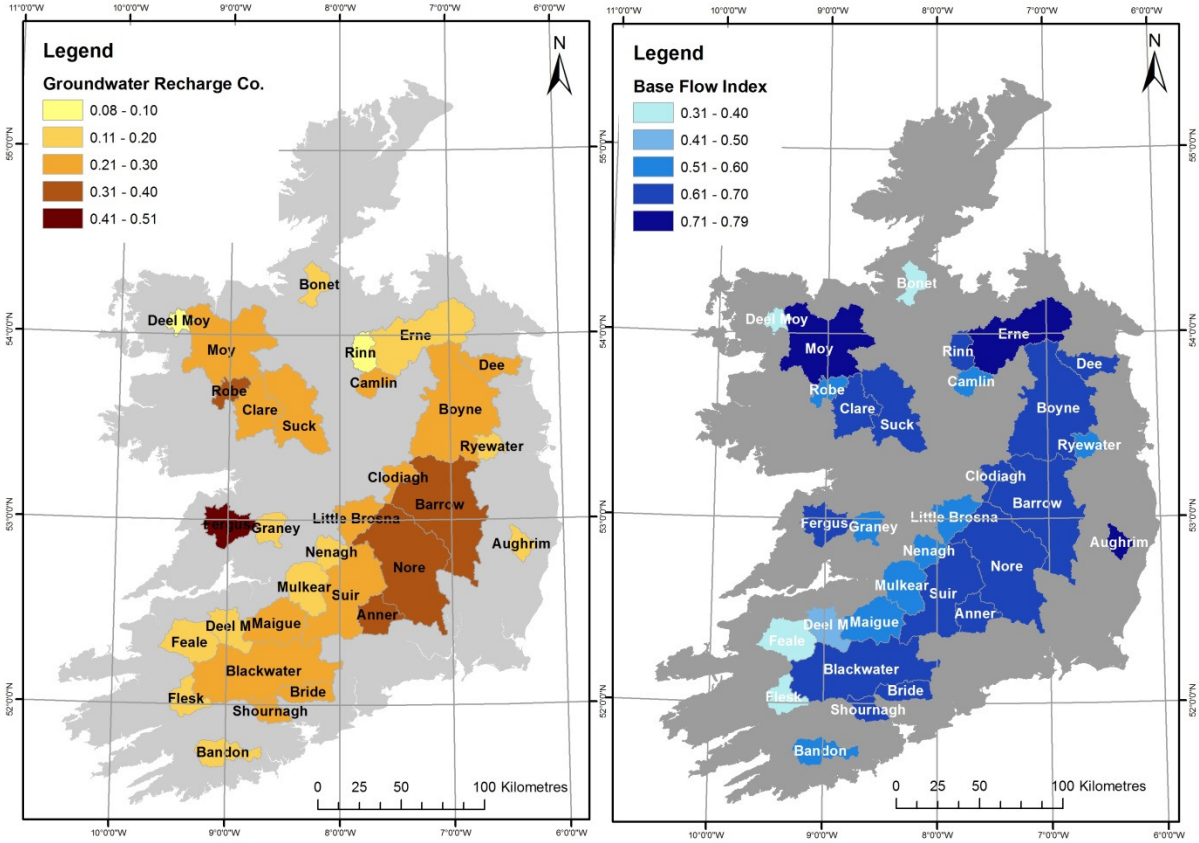

Figure 1. *Locations of 31 study catchments showing average groundwater recharge coefficient (left panel) and base flow index (right panel).*

2 METHODS AND MODELS

2.1 Uncertainty Analysis and Evaluation Criteria

For the three hydrological models, an uncertainty analysis was undertaken on their outputs for each of the 31 catchments (Figure 1) over the 16 year study period. Ensemble simulations were generated from the recommended model parameter ranges (see Mockler et al., 2015), assuming uniform probability distribution functions. Stratified sampling of these ranges using Latin Hypercube sampling generated $n(k+2)$ parameter sets where k is the number of model parameters and n is the base sample size (9,000 in this study). This resulted in 99,000, 108,000 and 117,000 simulations for the SMARG, SMART and NAM model, respectively.

In addition to analysis of the full set of sampled parameter sets, the best 1,000 simulations were selected for each model. These 'behavioural' parameter sets were identified based on the goodness of fit to the measured streamflows, using equal weighting of two criteria (detailed below). Similar Monte Carlo methods are frequently used to sample possible variations in inputs and parameters using assumed probability distribution functions e.g. the GLUE methodology (Beven and Binley, 1992). In this study, we used two performance criteria to quantify the adequacy of the simulation of total streamflow against the observed streamflow. The first is based on the Nash Sutcliffe efficiency (NSE) (Nash and Sutcliffe, 1970), a widely used goodness of fit measure based on the error variance defined as:

$$\mathbf{NSE} = 1 - \frac{\sum_{t=1}^{n}(Q_{o,t}-Q_{m,t})^2}{\sum_{t=1}^{n}(Q_{o,t}-\overline{Q_o})^2}$$

where $Q_{o,t}$ is the observed flow for time-step t, $Q_{m,t}$ is the modelled flow at time-step t, $\overline{Q_o}$ is the mean observed flow and n is the length of the time series. A bounded version of the Nash-Sutcliffe criterion (Mathevet et al., 2006) was calculated as:

$$C_{2M} = \mathrm{NSE} / (2 - \mathrm{NSE})$$

The C_{2M} criterion varies between -1 and +1 and results in lower positive values compared to NSE, thereby generating a less skewed distribution. The second criteria used is the mean residual error criterion (MR), which is an indicator of bias and is the difference between simulated and observed flows in the overall water balance i.e.:

$$\mathrm{MR} = \frac{1}{n}\sum_{t=1}^{n}(Q_{o,t} - Q_{m,t})$$

where $Q_{o,t}$ is the observed flow for time-step t and $Q_{m,t}$ is the modelled flow at time-step t. MR evaluates the overall water balance, whereas the NSE focuses on the correlation of the time series.

In addition to the criteria that assess streamflow simulations, a ratio of average groundwater contribution (GW_{avg}) to total streamflow was calculated for all simulations over the study period, as:

$$GW_{avg} = \frac{\frac{1}{n}\sum_{t=1}^{n}(GW_{m,t})}{\frac{1}{n}\sum_{t=1}^{n}(Q_{m,t})}$$

Where $GW_{m,t}$ is the modelled groundwater flow at time-step t.

2.2 Conceptual Rainfall Runoff Models

2.2.1 NAM Model

The 'Nedbør-Afstrømnings-Model' (NAM) model (Nielsen and Hansen, 1973) is an internationally established model, and has previously been used in Irish catchments for investigating the contributions of groundwater and surface water to streamflow (RPS, 2008, O'Brien et al., 2013, Mockler and Bruen, 2013). The NAM model has two storage reservoirs for soil moisture accounting and reservoirs representing four hydrological pathways (Figure 2 a). Some small amendments were made to reduce the original 15-parameter NAM model to a more parsimonious 11-parameter structure. These included (i) omitting the snow component from the structure, as it is not relevant to the Irish study catchments, (ii) relating the two quick flow routing parameters of two linear reservoirs in series to one parameter (SUPERCK), and (iii) fixing the groundwater contribution factor equal to one (following the assumption that groundwater transfers between catchments are negligible at this scale). Eight of these parameters control the moisture content in storages representing the surface, soil and groundwater storages, and three parameters relate to the routing components.

2.2.2 SMARG Model

The Soil Moisture Accounting and Routing with Groundwater component (SMARG) model was developed in NUI Galway (Khan, 1986, Kachroo, 1992, Tan and O'Connor, 1996). Its origins are in the layers model (O'Connell et al., 1970) and its water balance component is based on the 'Layers Water Balance Model' (Nash and Sutcliffe, 1970). The SMARG model has been widely applied in Irish catchments (Goswami et al., 2005, RPS, 2008, Bastola et al., 2011). SMARG has a soil moisture accounting component that represents the catchment as a vertical stack of soil layers. This component keeps account of the rainfall, evaporation, runoff, and soil storage processes using six parameters (Figure 2 b). When there is rainfall in a time step, the excess rainfall is calculated as the depth of water that exceeds potential evapotranspiration. This depth of water is used to calculate surface runoff, which is the sum of (i) direct runoff, (ii) infiltration excess, and (iii) a portion of saturation excess. The remainder of the saturation excess contributes to the groundwater, as determined by the groundwater weighting parameter (G). The routing component uses linear reservoirs with three parameters to simulate the attenuation effects of the catchment.

2.2.3 SMART Model Structure

The SMART model was developed to facilitate water quality modelling in Irish catchments, and was informed by the strengths of the SMARG and NAM structures. In this study it is used as a lumped conceptual model, although it can be used for semi-distributed modelling of catchments (Bruen and Mockler, 2012). The model has six soil layers of equal depth (Figure 2 c), similar to the SMARG, with six soil moisture accounting parameters. Drain flow is included as a separate flow path in the model, as this can be an important pathway for nutrients in agricultural catchments (e.g. Madison et al., 2014), and is related to soil moisture excess and the drain parameter (S), which varies between 0 and 1. Interflow is a combination of soil moisture excess and outflow from the soil layers, calculated using the soil outflow coefficient (D). Shallow and deep groundwater pathways are each calculated from individual outflow equations, also related to the outflow coefficient (D) parameter. Results from Sobol's variance based sensitivity analysis confirmed that the SMART model development reduced the number of poorly identifiable parameters, compared to the SMARG model (Mockler et al., 2015). Further details on the SMART model development are available in Mockler et al. (2014).

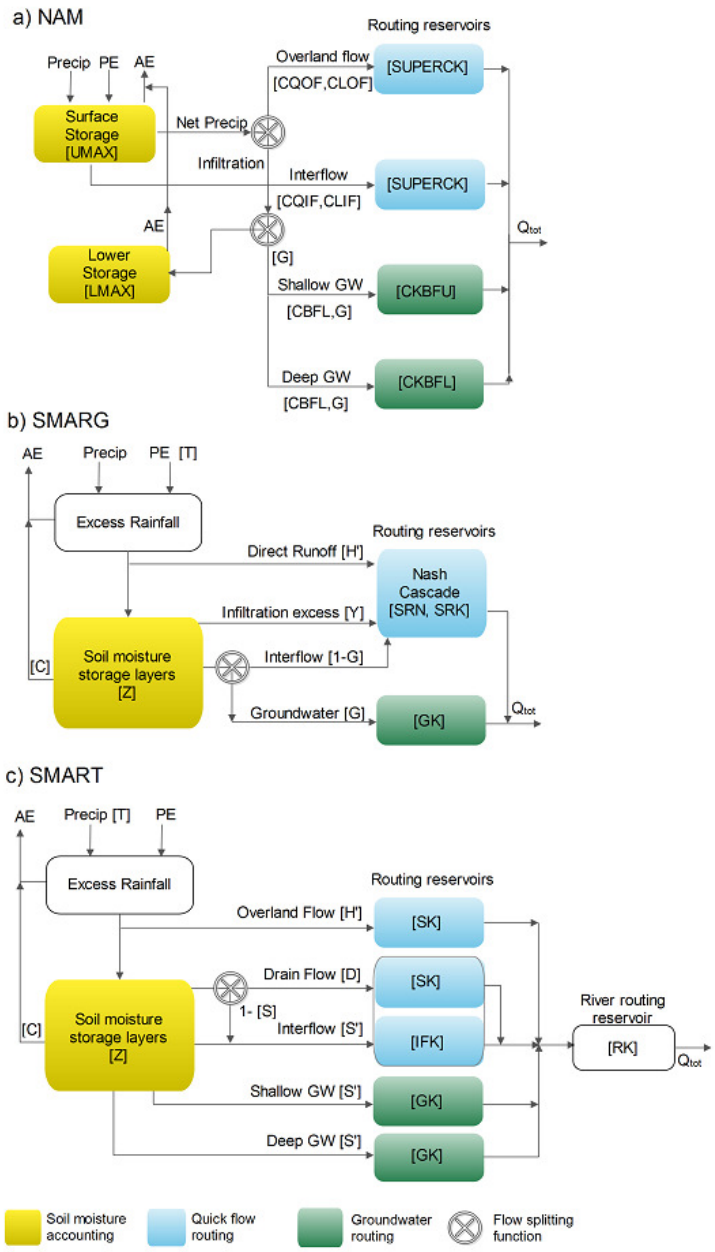

Figure 2. *Schematic representation of the NAM (a), SMARG (b) and SMART (c) models, with internal flow paths identified as either quick flow (blue) or groundwater (green).*

2.3 Study Catchments

The 31 study catchments (Figure 1) were selected on the basis of having good quality meteorological and hydrometric data available for the 16 year study period beginning from 1 January 1990. The chosen catchments cover over 35% of the country and represent a variety of meteorological and geological conditions across Ireland, with catchment areas ranging from 151 km^2 to 2460 km^2.

Meteorological data consisted of daily rainfall and potential evapotranspiration values obtained from the Irish meteorology office, Met Éireann. The catchment-area averaged rainfall was calculated using the Thiessen method, with each catchment using data from at least two precipitation stations and the

largest catchment (Boyne) containing 13 stations. Annual average rainfall (AAR) ranges from 820 mm in the Ryewater to 1897 mm in the Flesk with an overall average of 1189 mm. Potential evapotranspiration was obtained from ten stations distributed over the study area, with data from the nearest station selected for each catchment and assumed to be spatially uniform.

Hydrometric data for each catchment consisted of daily mean flows originating from the Irish Office of Public Works (OPW) and the Irish Environmental Protection Agency (EPA). Periods within the 16 years of the study with missing flow data at the catchment outlet were not included in the analysis. Of the 31 catchments, four have missing flow data for over 25 % of the study period, with the majority having less than 10 % missing values.

2.4 Catchment Groundwater Flow Indices

Groundwater is the part of the sub-surface water that is in the saturated zone, which typically flows through aquifers, although it can expand with increasing moisture conditions to include flow through the subsoils and soils. Two indices representing groundwater flow are used in this study to indicate proportion of groundwater contributing to streamflow in catchments:

1. The recharge coefficient (ReCo) is calculated from the Geological Survey of Ireland (GSI) groundwater recharge map (Hunter Williams et al., 2013), and does not incorporate any streamflow time-series. ReCo represents the deep groundwater resource in a catchment. The main hydrogeological properties used to generate the map were soil drainage properties, subsoil permeability and subsoil thickness. The limited ability of low permeability aquifers to accept percolating water is also taken into account by applying a maximum recharge capacity amount ('recharge cap'). For example, groundwater flow is predicted as low in areas overlain by thick, low permeability clay, and where low permeability aquifers are not able to accept percolating waters. ReCo is calculated as the predicted annual groundwater recharge (mm) as a percentage of the annual effective rainfall (mm).

2. The Base Flow Index (BFI) is a measure of the proportion of streamflow that is drawn from natural storages in the catchment. BFI is greater than the recharge coefficient as it can include flow through soils and subsoils. It was calculated from streamflow time-series by the Office of Public Works (OPW) using the 5-day minima method (Institute of Hydrology, 1980). The calculation of BFI has an intermediate step which calculates a BFI time series, which could be compared with modelled groundwater time series.

3 RESULTS & DISCUSSION

3.1 Hydrological Model Performance

Results from the simulations using the Latin Hypercube sampling parameter sets show that for each catchment, each model had some simulations that performed well at simulating streamflow, as evaluated by C_{2M} and MR. The mean C_{2M} results were 0.44, 0.18, 0.51 for the NAM, SMARG and SMART model, respectively, with results varying between catchments. The selection of parameter ranges and assumption of uniform distributions between these ranges have an influence on these results, and were guided by previous studies and literature. Sources of uncertainties in conceptual hydrological modelling results can arise in (i) model context, (ii) model structure, (iii) forcing data and (iv) parameters (Walker et al., 2003). The results presented in this paper assume that the model

context is sound and do not include uncertainty due to observed rainfall, potential evapotranspiration and streamflow time-series, in order to facilitate the focus on the model structure and internal flow partitioning.

Behavioural parameter sets were selected as the top 1,000 for each hydrological model from equal weighting of C_{2M} and |MR|, as evaluated against the observed flow data. The SMART model had the highest C_{2M} values, followed by the NAM and SMARG models (Table 1).

Table 1: *Summary of C_{2M} and MR results for the 31 catchments & correlation of GW_{avg} with catchment recharge coefficients (ReCo) and base flow indices (BFI) for 1,000 behavioural simulations for 3 models. The statistical significance is indicated by p-values (p).*

Model	C2M median (min, max)	MR median (min, max)	GWavg corr with ReCo	GWavg corr with BFI
NAM	0.6 (0.34,0.84)	0.01 (-0.19,0.2)	0.18 (p = 0.32)	0 (p = 0.98)
SMARG	0.59 (0.21,0.9)	0 (-0.32,0.19)	0.37 (p = 0.04)	0.66 (p = <0.001)
SMART	0.65 (0.39,0.85)	0 (-0.17,0.08)	0.45 (p = 0.01)	0.87 (p = <0.001)

3.2 Assessment of Groundwater Simulations

We further examined the 1,000 behavioural simulations for each hydrological model, with a focus on groundwater contribution to streamflow. It is noteworthy that the behavioural sets were not selected using an objective function that optimizes groundwater simulations, such as the NSE with log values. Rather, this study aimed to assess the groundwater contribution of simulations that would be suitable for a range of low to high flows, as is required in catchment simulations for water quality (Medici et al., 2012, Futter et al., 2014). Moreover, the simulations were not constrained by the groundwater indices (BFI or ReCo) that were used in this assessment, and instead were used as independent evaluators.

The median GWavg values for all catchments were 0.12, 0.33 and 0.42 for the NAM, SMARG and SMART models respectively. This large variation highlights the different flow partitioning of the models. All models identified at least one behavioural parameter set which resulted in no simulated groundwater. Figure 3 shows the distribution of GW_{avg} by hydrological model for the 1,000 behavioural sets, and for all model simulations using Latin Hypercube sampling. For each model, the distribution of GW_{avg} for the total number of sampling sets and the 1,000 behavioural sets are broadly similar. These highlight that the majority of NAM model simulations have a lower contribution of groundwater than is indicated by both the ReCo, which represents the deep groundwater, and the BFI, which represents total base flow contributions. The distributions of GW_{avg} for the SMARG and SMART models are more closely aligned with the ReCo and BFI values.

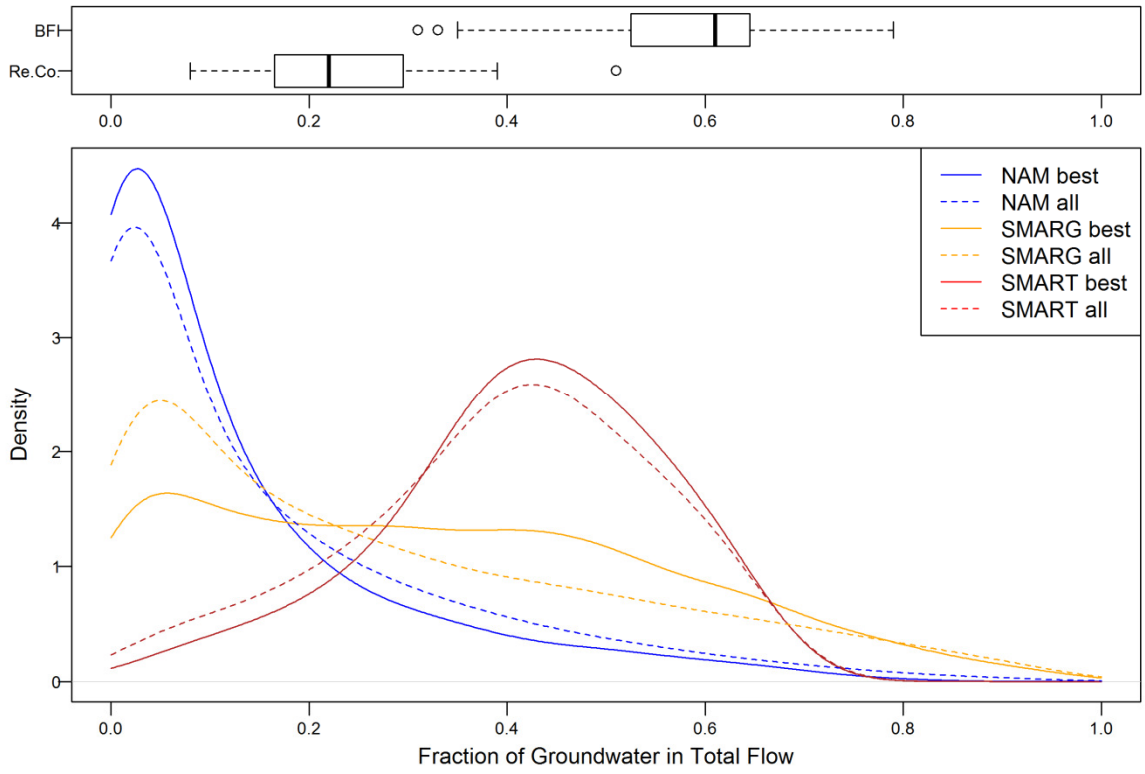

Figure 3. *Distribution of the fraction of groundwater contributing to total flow for 31 catchments from NAM (blue), SMARG (yellow) and SMART (red) for all model simulations ('all'; dashed line) and behavioural sets ('best'; solid line) using Latin Hypercube sampling of standard parameter ranges with uniform distributions The distributions of BFI and ReCo indices from measured data are shown at the top of the Figure.*

The internal flow partitioning for each catchment was notably different across the models. To demonstrate this, the percentage of groundwater contributing to simulated streamflow was compared with catchment groundwater flow indices. Correlations between GW_{avg} results and the BFI and ReCo (defined in Section 2.2) indicate whether the internal hydrological processes of the models are aligned with the understanding of processes from catchment characteristics. Of the three models, the SMART model had the strongest correlations with ReCo and BFI values across the catchments (Table 1). This indicates that the processes of SMART that produce quick in-stream responses and groundwater flow are more representative of what is expected from catchment characteristics.

The range of simulated GW_{avg} for each catchment produced by the 1,000 simulations indicated the degree of uncertainty in attributing flow to quick flow or groundwater. The SMARG had the highest prediction ranges, which tended to increase with increasing BFI i.e. greater uncertainty in groundwater dominated catchments. The SMART model produced the lowest ranges of GW_{avg} estimates (Table 1), indicating that the SMART model has less uncertainty simulating internal processes.

There is a growing body of literature highlighting the importance of assessing model structure adequacy (Wagener et al., 2001, Clark et al., 2008, Gupta et al., 2012). In this study, the three conceptual models have different representations of surface runoff (or quick flow) and groundwater contributions to streamflow. All three models assume that the surface water and groundwater of the study catchments aligned, and that there are no transfers into or out of the catchment. This assumption

may not be true, particularly for catchments with extensive subsurface paleochannels crossing catchment boundaries, or conduit karst aquifers i.e. Clare, Fergus, Robe and Suck catchments. The NAM and SMART models have more detailed internal flow partitioning compared to the SMARG model, and therefore are less flexible to adapt to different hydrological conditions. In particular, the modelled internal flow paths of catchments with conduit karst aquifer bedrock may need to be interpreted, where, for instance, a simulated quick flow path is actually representing the groundwater conduit flow.

4 CONCLUSIONS

For coupled water quantity and water quality modelling, a hydrological model is required that can capture both the total flows and the groundwater contributions to streamflow. A comparison of results from Monte Carlo simulations of 31 study catchments for the NAM, SMARG and SMART models highlight that the relative contribution of groundwater estimated by each model depends on both the model structure and the catchment characteristics. Internal flow partitioning varies greatly between models and, to varying degrees, between behavioural parameter sets for each model. This study illustrated this by comparing the simulated annual groundwater contributions to streamflow with additional independent information, in the form of groundwater flow indices.

Results show that the new SMART model performed better than two established models, NAM and SMARG, at representing both the total streamflow and the indicators of internal flow paths (BFI and ReCo) of the 31 Irish study catchments. Many other popular models could be compared in a similar manner, including GWLF (Schneiderman et al., 2002) and SWAT (Arnold et al., 1998). However, the key point is that groundwater and surface water interactions simulated by any selected model and parameters must be critically assessed when coupling with water quality modelling. In additional, information on plausible groundwater flow contributions should be incorporated into model calibration. Ideally, water quality models should include ensembles based on behavioural parameter sets that incorporate ranges of feasible flow partitioning.

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