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Regionalization of hydrological models for flow estimation in ungauged catchments in Ireland

Saeed Golian *, Conor Murphy, Hadush Meresa

Irish Climate Analysis and Research UnitS (ICARUS), Department of Geography, Maynooth University, Maynooth, Co. Kildare, Ireland

A R T I C L E I N F O

Keywords:
Regionalization
Hydrologic models
High flows
Low flows
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A B S T R A C T

Study Region: The study area consists of 44 catchments across Ireland.
Study Focus: We regionalize two hydrological models (GR4J and GR6J) to produce continuous discharge simulations and compare performance in simulating high, median and low flow conditions with other established approaches to prediction in ungauged basins and a simple benchmark of using the median parameter set across all catchments. These include K-nearest neighbor (KNN) and statistical methods for predicting flow quantiles using catchment characteristics. Different objective functions were selected for different parts of flow regime and the success of different methods for regionalizing hydrological model parameters; including multiple linear regression (MLR), non-linear regression (NL) and random forests (RF) were evaluated.
New Hydrological insights for the Region: All regionalization approaches perform well for average flow conditions. The GR4J model regionalized using RF performs best for simulating high flows, though all regionalized models underestimate the median annual flood. GR6J regionalized using RF performs best for low flows. While KNN and statistical approaches that directly leverage physical catchment descriptors provide comparable median performances across catchments, the spread in relative error across our sample is reduced using regionalized hydrological models. Our results highlight that the choice of hydrological model, objective functions for optimization and approach to linking model parameters and physical catchment descriptors significantly influence the success of regionalization for low and high flows.

1. Introduction

The challenge of flow estimation in ungauged catchments has been the focus of much research in hydrology (e.g. Razavi and Coulibaly, 2013; Sivapalan, 2006). Various regionalization techniques ranging from empirical methods to estimate parameters of the statistical distribution of discharge (e.g. flood frequency distribution or flow duration curve), to continuous simulation of discharge time series through application of hydrological models to ungauged catchments have been developed (He et al., 2011). At the core of these methods is the transfer, or regionalization, of hydrological information from gauged to ungauged catchments. Of the available methods, three robust and widely used regionalization approaches are: i) spatial similarity methods, e.g. spatial proximity, ii) statistical/mathematical-based approaches e.g. regression-based methods and, iii) physical similarity approaches (Samuel et al., 2011; Arsenault et al., 2019). The differences between approaches lie in the type of information that is transferred from gauged to ungauged catchments, the transfer method and the catchment properties used to quantify similarity (Pagliero et al., 2019). Oudin et al. (2008)

* Corresponding author.
E-mail address: saeed.golian@mu.ie (S. Golian).

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compared different regionalization methods over catchments in France and found that spatial proximity methods provide the best regionalization solution for their study catchments. Li et al. (2014) compared two methods based on spatial and physical similarity, to regionalize parameters of two hydrologic models for catchments in the Tibetan Plateau. They found that spatial proximity slightly outperformed the physical similarity method.

While many efforts have been made to regionalize streamflow characteristics, e.g. flood peaks (Hailegeorgis and Alfredsen, 2017) and low flow (Longobardi and Villani, 2008; Salinas et al., 2013), the majority of efforts are devoted to streamflow regionalization using hydrological models (Razavi and Coulibaly, 2013). Conceptual hydrological models are a popular means of simulating continuous flow estimates at gauged catchments due to low input data requirements, typically only needing precipitation and temperature/potential evapotranspiration, together with calibrated model parameters to simulate flow. These models have also been shown to be equally reliable as more complex physically based models for simulation in ungauged catchments (Yadav et al., 2007). For calibration, observed discharge data are necessary to identify values for parameters that define the conceptual structure of the model for runoff generation and routing. Due to the limited availability of discharge data for model calibration, applying hydrological models to catchments with no existing observations is a fundamental challenge for hydrologists (Wagener et al., 2004; Takeuchi, 2007; Amiri et al., 2016).

Attempts to regionalize hydrological model parameters for prediction in ungauged catchments have been made in a wide variety of contexts, with the majority of studies using linear regression to relate calibrated model parameters to physical catchment characteristics describing the climate and hydrological conditions of the catchment. For instance, Yokoo et al. (2001) used multiple linear regression to establish the relationship between parameters of the calibrated TANK model (Sugawara, 1995) and catchment characteristics. They applied their method to 12 catchments in Japan and found that TANK parameters can be satisfactorily regionalized based on physical properties of the catchments. In the UK, Young (2006) examined two methods to regionalize hydrological model parameters including, a regression-based method to relate model parameters to catchment characteristics and a nearest-neighbor approach using calibrated parameter sets from a large dataset of 260 catchments, concluding that regression-based methods resulted in better performance in simulating river flow. Also in the UK, Deckers et al. (2010) attempted to regionalize the parameters of the HBV model using regression to relate optimized parameter sets to catchment characteristics, finding that such attempts did not outperform default parameter values for simulating in ungauged catchments. Song et al. (2019) used a multiple regression model to derive relationships between calibrated parameters of the TANK model and watershed characteristics in South Korea. While their results showed acceptable accuracy of the resultant regionalized model (i.e. NSE > 0.5 and $|PBias| \leq 15\%$), they emphasized that the uncertainties associated with calibration of model parameters could largely affect the accuracy of regionalization. Arsenault et al. (2019) applied three regionalization methods to derive parameter sets for hydrological models including, multiple linear regression, spatial proximity and physical similarity for predicting streamflow at 30 diverse catchments in Mexico. They applied three hydrological models, namely GR4J (Perrin et al., 2003), HMETS (Martel et al., 2017) and MOHYSE (Fortin and Turcotte, 2007) and deduced that model performance for arid catchments was worse in the context of regionalization, with GR4J being more robust than the other models due to its simpler structure.

By contrast, fewer studies have employed non-linear and/or machine learning methods to regionalize hydrological model parameters. Heuvelmans et al. (2006) used Artificial Neural Networks (ANNs) to regionalize the SWAT model in a Flemish catchment, concluding that ANNs outperformed linear regression methods and were better able to represent the non-linear relationship between catchment characteristics and model parameters. Saadi et al. (2019) examined the potential application of the random forest (RF) method to regionalize the GR4J hydrologic model using catchment descriptors, finding that the performance of RF compared favorably to two benchmark methods based on proximity and similarity. In another effort, Brunner et al. (2018) compared three nonlinear regression methods for regionalization of synthetic design hydrographs, concluding that nonlinear approaches resulted in better performance than linear regression.

In Ireland, approaches to regionalization have been based on the use of statistical methods and physical similarity to relate catchment descriptors to low and high flow statistics, with few if any published attempts to regionalize a hydrological model for continuous simulation in ungauged catchments. For example, Murphy (2009) used physical catchment descriptors to directly simulate the median annual flood (QMED) in ungauged catchments. Mandal and Cunnane (2009) developed a regression based method to predict quantiles of the flow duration curve for ungauged catchments from catchment descriptors, while Bree (2018) used a region of influence approach employing catchment descriptors to transfer estimates of the flow duration curve based on hydrological similarity.

We attempt to regionalize conceptual hydrological models for continuous streamflow estimation in Irish catchments. In doing so, we examine the application of i) multiple linear regression (MLR), ii) non-linear regression (NL), and iii) random forests (RF) for relating model parameters to available catchment characteristics. Given our focus on simulating the full flow regime we incorporate different objective functions (OFs) for calibration of the hydrological models prior to regionalization. We evaluate performance of our regionalized conceptual rainfall-runoff (CRR) models in simulating key metrics representing high, medium and low flows against a simple benchmark (median calibrated parameter set across our catchment sample) and widely used alternative strategies including; i) the transfer of information from physically/hydrologically similar catchments using a K-nearest neighbor approach and; ii) previously established statistical methods for estimating floods and quantiles of the flow duration curve directly from catchment characteristics. Finally, we relate the relative error in simulating flow characteristics to catchment physiographic and climatic attributes. The remainder of the paper is organized as follows. Section 2 provides information on the data and methods used. Results are presented and discussed in Section 3, before we distil key conclusions in Section 4.

2. Data and methods

Our study design is illustrated in Fig. 1. For our sample of 44 catchments across Ireland, each regionalization method (Statistical, K-nearest neighbor (KNN) and CRR model regionalization) are applied and compared in simulating high, median and low flow characteristics. For each catchment the ability of different methods to simulate high flows is evaluated using Qmed (median of daily annual maxima flow series), while for median and low flows Q50 and Q95 (the 50th and 95th exceedance probability flow values from the flow-duration curve) are used. We take simulations of each indicator obtained using the median optimized hydrological model parameter set derived across all catchments as a benchmark against which different regionalization approaches are evaluated.

Our statistical method adopts and modifies regression based approaches previously developed for flow estimation in ungauged catchments in Ireland. For KNN, physiographical and climatic characteristics of catchments are used to simulate discharge based on K-nearest gauged neighbors with similar characteristics to the catchment under investigation. Finally, for regionalizing hydrologic models, the parameters of two parsimonious conceptual hydrological models (GR4J and GR6J) are optimized for 44 catchments. We then use regression and machine learning approaches to link model parameters to physical catchment descriptors (PCDs) before simulating different components of the flow regime.

2.1. Catchment sample and physical descriptors

Daily discharge for each of the 44 catchments (Fig. 2) were obtained from the hydrometric data portals of the Office of Public Works (OPW) (https://waterlevel.ie/hydro-data/home.html) and the Environmental Protection Agency (https://www.epa.ie/hydronet/). To derive the necessary input to our hydrological models, we used gridded (1 × 1 km) daily precipitation and temperature data (Walsh, 2012), area averaged for each catchment. Daily potential evapotranspiration was estimated from air temperature and radiation using the method of Oudin et al. (2005) as more physically based methods (e.g. Penman-Monteith) are not available for all catchments, given their larger data requirements.

Physical catchment descriptors (PCDs) for each catchment were obtained from the OPW's Flood Study Update (FSU; http://opw.hydronet.com; Mills et al., 2014). PCDs provide information on the morphometric, soil and climatological properties of each catchment. Table S1 provides an overview of the PCDs employed and their units of measurement, while Table S2 provides a breakdown of PCDs for all 44 catchments. Fig. S1 shows the correlation matrix for all PCDs. There are some strong correlations between PCDs (e.g. strong negative correlation between SAAPE and FLATWET, and very strong positive correlation between ARTDRAIN and ARTDRAIN2 and between STMFRQ and NETLEN), consequently, the prevalence of collinearity between selected predictors was noted in building regression models (see Section 2.2). Relative to a larger sample, the catchments used are representative of different hydro-climatological conditions across the island, but with a recognized under inclusion of smaller upland catchments located along coastal margins (Broderick et al., 2019).

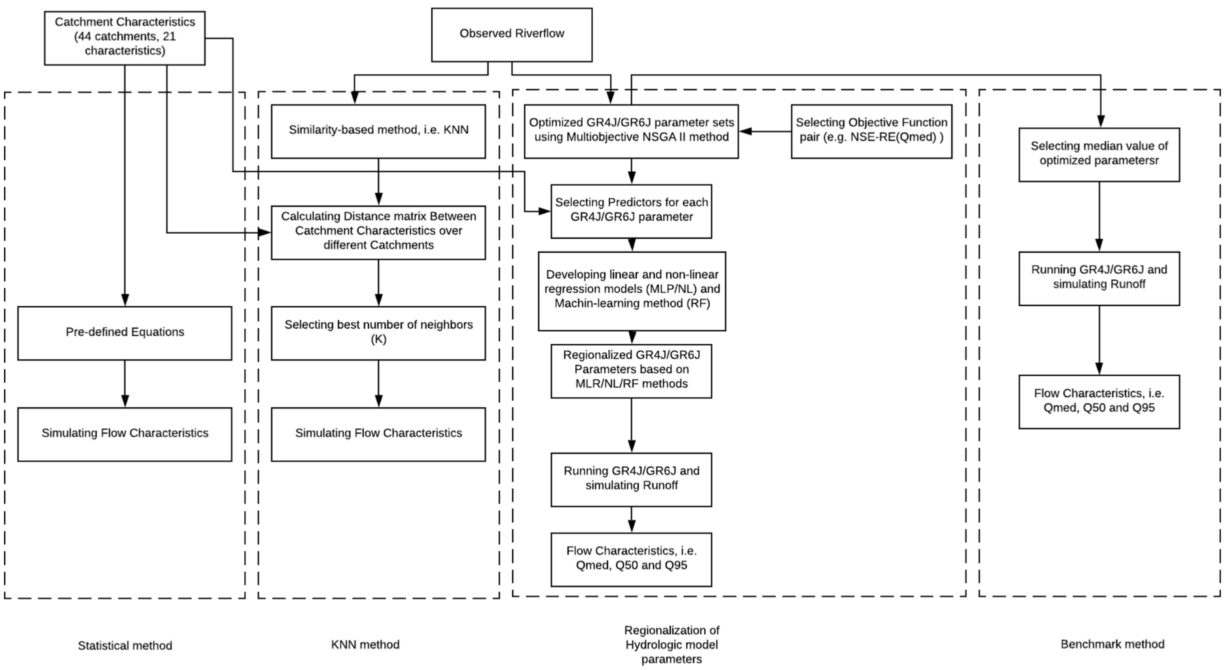

Fig. 1. Flowchart of the regionalization methodology employed.

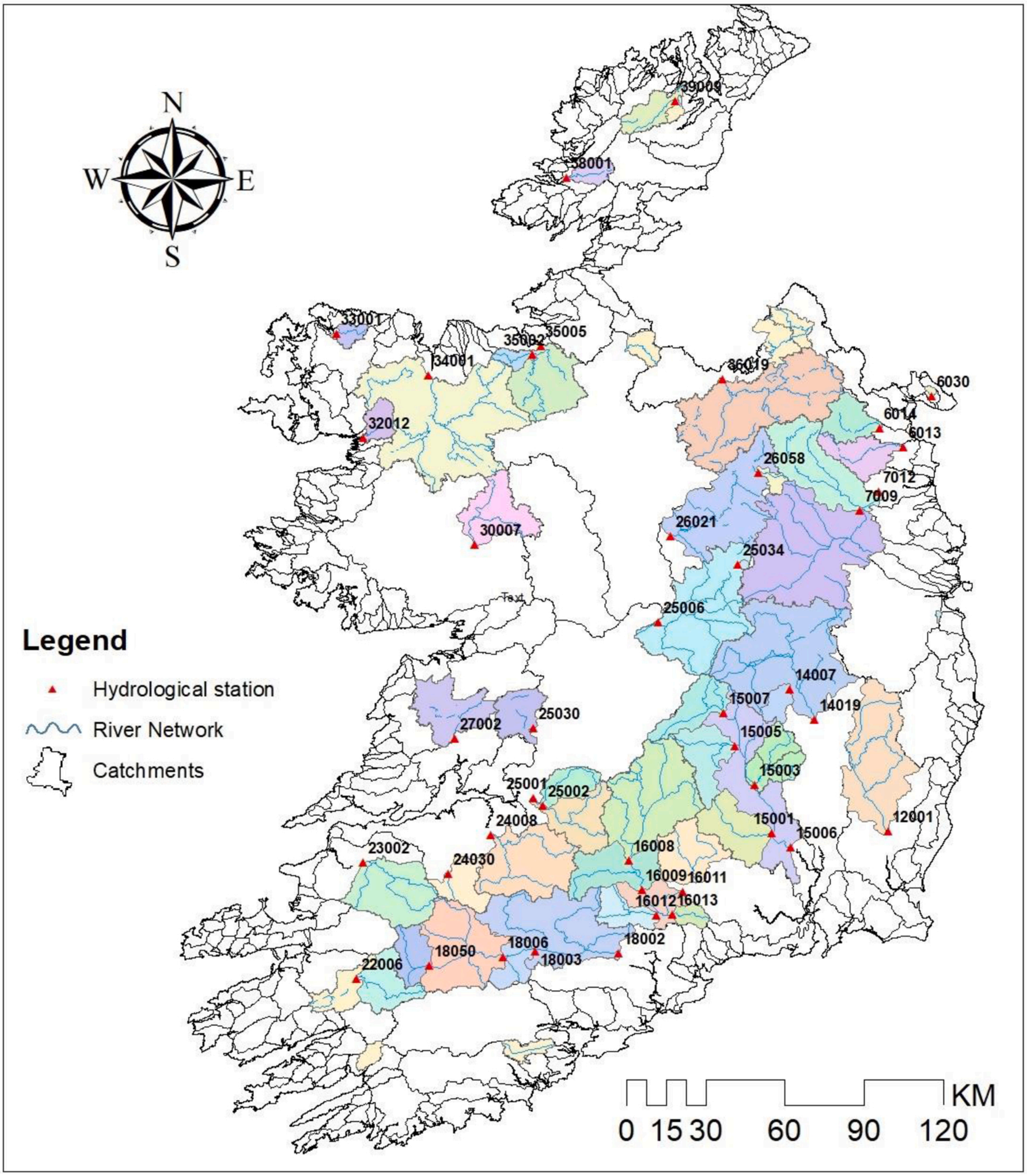

Fig. 2. Location of the 44 catchments selected for this study.

2.2. Hydrological models

We employ the GR4J and GR6J hydrological models developed as part of the airGR R hydrological modelling package version 1.4.3.60 (Coron et al., 2017). Fig. S2 shows the schematic representation of the GR4J and GR6J models. Both GR4J/GR6J are simple lumped, two-/three-storage conceptual rainfall-runoff models that take precipitation (P) and potential evapotranspiration (PE) as inputs. GR6J contains six parameters (GR6J); X1, the maximum soil moisture storage (mm); X2, the groundwater exchange coefficient (mm/day); X3, the maximum capacity of the routing storage (mm); X4, the time peak ordinate of hydrograph unit UH1 or flow delay (day), X5, groundwater exchange threshold (-) and X6, exponential store controlling parameter (mm) (in parallel with X3). If parameters X5 and X6 neglected, GR6J reduces to GR4J by modification of corresponding groundwater exchange functions (Perrin et al., 2003; Pushpalatha et al., 2011). These models have previously been used for regionalization in several studies (e.g. Drogue and Khediri, 2016; Qi et al., 2020).

To optimize the parameters of the hydrological models, we applied the Non-dominated Sorting Genetic Algorithm (NSGA-II) method (e.g. Guo et al., 2014; Huo et al., 2016), a multi-objective optimization algorithm developed by Deb and Goel (2001; Deb et al. (2000). Seventy percent of data were used for calibration of model parameters and 30 percent for validation. We identify three different sets of parameters for each catchment for simulating high, median and low flows. Consequently, we used three pairs of objective functions namely, Nash-Sutcliffe and relative error (RE) in simulating Qmed (NSE-RE(Qmed)), Nash-Sutcliffe based on log-transformed simulated flow and RE in simulating Q95 (logNSE-RE(Q95)) and finally the non-parametric Kling Gupta efficiency (npKGE) and RE for simulating Q50 (npKGE-RE(Q50)).

The Nash-Sutcliffe Efficiency (NSE) is calculated using the following equation (Nash and Sutcliffe, 1970):

$$NSE = 1 - \frac{\sum_{t=1}^{n} \left(Q_{t,o} - Q_{t,s}\right)^2}{\sum_{t=1}^{n} \left(Q_{t,o} - \overline{Q}_{obs}\right)^2} \tag{1}$$

Where $Q_{t,o}$ and $Q_{t,s}$ are observed and simulated flow at time t, $\overline{Q}_{obs}$ is average observed flow and n is number of observations. *logNSE* is the same as *NSE*, but flows are log-transformed before applying Eq. 1.

The KGE goodness-of-fit measure was developed by Gupta et al. (2009) to provide a diagnostically useful decomposition of the NSE (and hence MSE), which facilitates the analysis of the relative importance of its different components. In this research, we used the non-parametric KGE (npKGE), calculating three components namely, r_s, β and α_{NP} as in Eqs. 2–5 (Pool et al., 2018). In comparison to ordinary KGE, non-parametric KGE meets assumptions regarding data linearity, normality, and the absence of outliers (Pool el at., 2018).

$$npKGE = 1 - \sqrt{(r_s - 1)^2 + (\beta - 1)^2 + (\alpha_{NP} - 1)^2} \tag{2}$$

$$\beta = \frac{\overline{Q}sim}{\overline{Q}obs} \tag{3}$$

$$\alpha_{NP} = 1 - 0.5 \sum_{k=1}^{n} \left| \frac{Q_{sim}(I(k))}{n\overline{Q}_{sim}} - \frac{Q_{obs}(J(k))}{n\overline{Q}_{obs}} \right| \tag{4}$$

$$r_s = \frac{\sum_{t=1}^{n} (Q_{obs}(t) - \overline{Q}_{obs})(Q_{sim}(t) - \overline{Q}_{sim}) -}{\sqrt{(\sum_{t=1}^{n} \left(Q_{obs}(t) - \overline{Q}_{obs}\right)^2)(\sum_{t=1}^{n} (Q_{sim}(t) - \overline{Q}_{sim})^2)}} \tag{5}$$

Where r_s is the Spearman rank correlation, $I(k)$ and $J(k)$ are the time steps when the k th largest flow occurs within the simulated and observed times series, respectively. $\overline{Q}_{obs}$ and $\overline{Q}_{sim}$ are the average flow for observed and simulated datasets, respectively. Both NSE and npKGE efficiencies range from $-\infty$ to 1. Essentially, the closer to 1, the more accurate the model is.

2.3. Regionalization methods

2.3.1. Regionalization of hydrological model parameters

2.3.1.1. Multiple linear regression (MLR) and non-linear regression (NL) methods. Linear and non-linear regression methods aim to fit a linear/non-linear model between optimized parameters of GR4J and GR6J as target (predictant) and PCDs as potential predictors. Here, an exhaustive search method was used to evaluate all possible combinations of predictor variables and select the best combination(s) based on pre-defined performance criteria, R^2 in this research. Potential multicollinearity between the explanatory variables in the final regression models was assessed using the Variance Inflation Factor (VIF) to avoid redundancy between predictor variables (Fox and Monette, 1992). Based on selected predictors, the coefficients were calculated using leave one out cross-validation (LOOCV). In this method, first one catchment is left out and the regression model is calibrated based on the remaining 43 catchments and the error associated with prediction is recorded. This procedure is repeated for all catchments and the overall prediction error is computed as the average of all test error estimates.

2.3.1.2. Machine learning: random forest. Random Forest (RF) is a machine learning method developed by Breiman (2001) which uses bagging (bootstrapping) to build a possible matrix of solution trees with uniform variance to produce accurate predictions of the dependent variable (Naghibi et al., 2017). RF has been widely applied in hydrology due to its flexibility, generalization and stability (Were et al., 2015). Cutler et al. (2007) used RF for ecological classification using plant species data, while Broderick et al. (2019) applied RF for catchment classification, highlighting the proficiency of the method in identifying group membership. Booker and Woods (2014) used RF for predicting hydrological indices in ungauged catchments, producing reasonable regression trees between hydrological indices and Generalize Extreme Value (GEV) parameters. In this study, we applied RF to develop a decision tree for each of the hydrological parameters describing the GR4J/GR6J models as a function of 21 PCDs across 44 catchments (Table S2). First, we split the full multidimensional matrix into two groups, i.e. two thirds (19) of the catchments were used for training the RF method and the remaining for checking the stability of the RF parameters and validation. Out of the 44 by 19 multidimensional matrix, we combined possible randomly selected decision trees into an assemblage to select the best combination of independent and dependent variables by testing different subset samples from the training matrix. The selection of features is derived from the random sampling of input matrix data sets and derived regression trees. A portion of the samples left out from the full matrix dataset and called out-of-bag samples (OOBS) were used to train and test the RF model. In the process of OOBS, we also optimize two important parameters of the RF algorithm: the number of trees considered in the forest and number of variables that fully describe the target (predictor). We used the coefficient of determination (R^2) to minimize the model error for each tree during the OOBS process and to evaluate performance.

2.3.1.3. K-nearest neighbor method (KNN). The KNN method is categorized as a physical similarity regionalization method whereby catchments with similar attributes (i.e. PCDs) are assumed to have similar hydrological behavior. Using a distance measure as a function of differences between PCDs, here Euclidean distance (Eq. 7), K catchments with least distance (most similarity) to the catchment under investigation are selected to calculate the flow characteristic as follows:

$$dist(C_i, C_j) = D_{i,j} = \sqrt{\sum_{r=1}^{m} \left(PCD_{i,r} - PCD_{j,r}\right)^2} \tag{6}$$

where $dist(C_i, C_j)$ or $D_{i,j}$ is the distance between catchments C_i and C_j, PCD_i and PCD_j are normalized characteristics for catchments i and j and m is the number of characteristics.

$$Q_m = \sum_{i=1}^{K} \frac{{}^{1}/D_{i,m}}{\sum_{j=1}^{n} {}^{1}/D_{j,m}} Q_i \tag{7}$$

where Q_m is the estimated flow characteristics at catchment m, $D_{i,m}$ is the distance between catchments C_m and C_i, Q_i is the flow characteristic at catchment i and K is the number of nearest neighbors which should be taken into account. LOOCV is applied to the KNN method. First one catchment is left out and the associated error for KNN method based on the remaining 43 catchments is recorded. This procedure is repeated for all catchments and the overall prediction error is computed as the average of all test error estimates. The performance of the KNN method is affected by the number of selected neighbors (K); here K is determined by trial-and-error so that the minimum root mean square error (RMSE) in simulating flow characteristics is derived.

2.3.1.4. Statistical equations. Two previously defined statistical approaches to estimating flows in ungauged catchments in Ireland were also incorporated into our assessment. Both establish a statistical relationship between flow features and selected catchment characteristics which can be generalized to ungauged catchments. According to Mandal and Cunnane (2009), p-percentile flow can be estimated using the following equation:

$$Q_p = \left(0.0229e^{0.1393(\mathrm{Ln}\,AREA)(\mathrm{Ln}\,SAAR)}\right) * (4.6558 - \mathrm{Ln}(p)) \tag{8}$$

Where Q_p is the p-percentile (%) flow, $AREA$ is catchment area (km^2), $SAAR$ is the long-term (1961–1990) average annual precipitation (mm) and Ln(.) is the natural logarithm. To estimate Q_{50} and Q_{95}, p should be equal to 50 and 95 percent, respectively. As part of the Flood Studies Update for Ireland, Murphy (2009) developed a statistical approach using catchment descriptors to estimate Qmed (median annual maximum flow) derived from instantaneous (15 min) annual maxima for ungauged catchments. To calculate Q_{med} in this research we modify the Murphy (2009) equation by re-calibrating the coefficients of the same model structure using annual maxima series derived from daily mean flows, returning the following model for estimating Qmed from PCDs (Murphy, 2009);

$$Q_{med} = 1.082 \times 10^{-2} AREA^{1.142} BFIsoil^{-0.191} SAAR^{0.196} FARL^{3.462} DRAIND^{0.943} S1085^{0.312} (1 + ARTDRAIN2)^{0.0951} \tag{9}$$

Where $BFIsoil$ is the baseflow index derived from soils, $FARL$ is an index of flood attenuation, $DRAIND$ is drainage density (km. km^2), $S1085$ is slope of main-stream (m/km) and $ARTDRAIN2$ is proportion of river network length included in Arterial Drainage Schemes.

2.4. Performance assessment

To assess the performance of different methods in simulating derived flow indices, i.e. Qmed, Q50 and Q95 we derived the relative error as follows:

$$RE\ (\%) = \frac{(Qmed_o - Qmed_s)}{Qmed_o} \times 100 \tag{10}$$

Where $Qmed_o$ and $Qmed_s$ are observed and simulated Qmed. Qmed is replaced with Q50 and Q95 to evaluate the performance of methods for medium and low flow conditions, respectively. The closer RE is to zero, the better the model performance; positive (negative) RE reflects underestimation (overestimation) of the target flow values. Finally, using derived REs a correlation analysis was also performed to evaluate errors associated with all methods for different catchment types. Statistical significance was evaluated at the 5% significance level.

3. Results

3.1. Hydrological model optimization

Optimized parameters for both the GR4J and GR6J models were evaluated in simulating Qmed, Q50 and Q95 for the validation period using relative error (RE) compared with observed values. A summary of model performances for all catchments is provided in Tables S3 and S4. Fig. 3 shows how multi-objective optimization improves the performance of both models in simulating flow characteristics compared to the uni-objective function (uni-OF) case. It can also be seen that using a single OF (uni-OF), on average across the sample of catchments, GR6J outperforms GR4J. Fig. 4 shows boxplots of RE in simulating Q50, Q95 and Qmed for each catchment and GR model using different multi-OF pairs. For both GR4J and GR6J, while all OFs resulted in satisfactory performance in simulating Q50, npKGE-RE(Q50) performs slightly better. For Q95 and Qmed, logNSE-RE(Q95) and NSE-RE(Qmed) led to much better performance in simulating low- and high-flow characteristics, respectively. Relative to GR4J, GR6J performs slightly better, especially in simulating low-flow conditions, i.e. Q95 based on logNSE-RE(Q95), however the difference between models is not significant. Fig. S3 shows the spatial distribution of RE for optimized GR4J and GR6J model. It can be seen that both models perform satisfactorily over all catchments with REs in the ±10% for approximately all catchments. Henceforth, we show results for low, medium and high flow conditions derived using logNSE-RE(Q95), npKGE-RE(Q50) and NSE-RE(Qmed) respectively.

3.2. Regionalization of hydrological model parameters

Regionalization of hydrologic model parameters using MLR and NL methods began by selecting the best combination of predictors (PCDs) for the parameters of each GR model, i.e. X_i, $i = 1, \ldots, 4$ for GR4J model and $i = 1, \ldots, 6$ for GR6J in simulating low, median and high flows. The model predictors selected following an exhaustive search are presented in Tables 1 and 2 for GR4J and GR6J models,

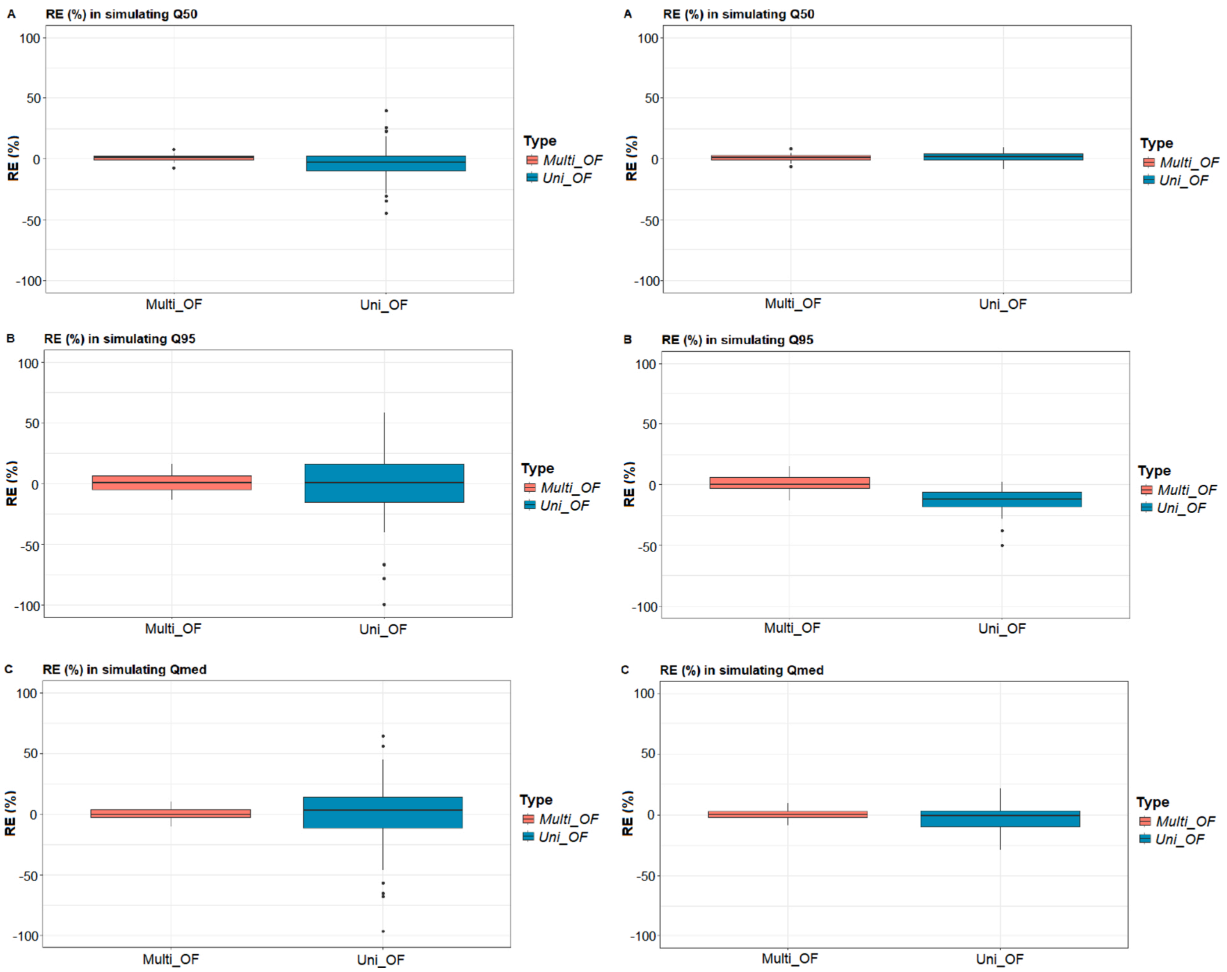

Fig. 3. The RE of simulated flow characteristics based on different Objective Functions (OFs) a) npKGE-RE(Q50) and npKGE b) logNSE-RE(Q95) and logNSE and c) NSE-RE(Qmed) and NSE for Multi-OF and uni-OF respectively. The left column represents GR4J and right are GR6J results.

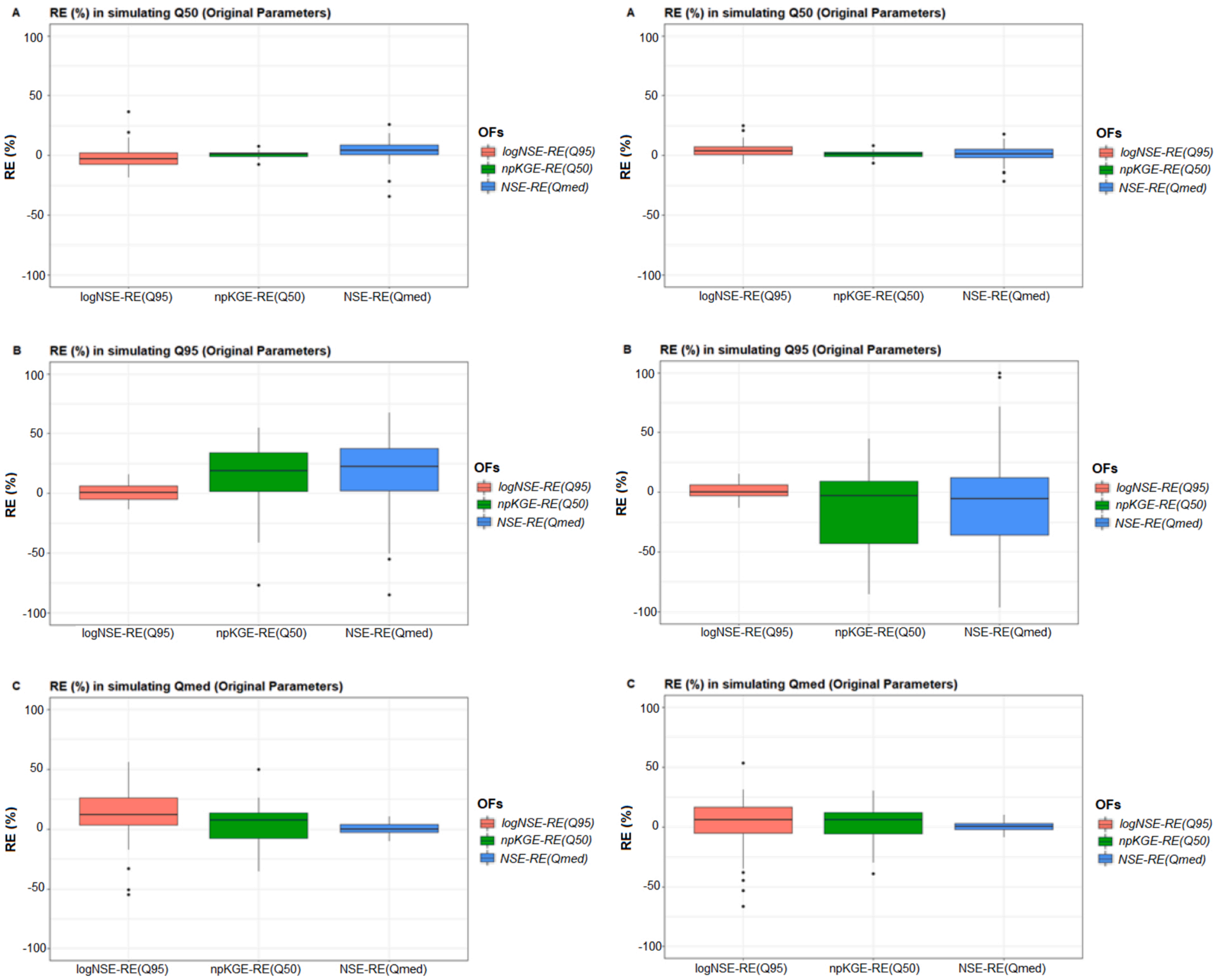

Fig. 4. Boxplots of relative error (RE) over study catchments based on different objective functions (OFs) in simulating a) Q50, b) Q95 and c) Qmed using the GR4J model (left column) and GR6J model (right column).

respectively. For the RF method, all PCDs are used given the robustness of the method to multicollinearity. Based on different OFs, different sets of predictors are returned for MLR and NL methods for an identical GR4J/GR6J parameter as predictand. The number of selected predictors using MLR method varies from 1 to 5 for different cases, i.e. OFs and predictand (model parameter). For the NL method, the number of selected predictors are higher, resulting in more complicated non-linear equations. Table 3 contains the performance of different regionalization methods in regionalizing parameters of the hydrologic models. RF exhibited the best performance, i.e. higher R^2 and lower RMSE values compared to MLR and NL methods for both models and the target flow metrics. The only exceptions are for X2 in medium flow regime for both GR4J and GR6J model where MLR provides better results and for X2 in high-flow regime for GR6J model where NL slightly outperforms RF.

3.3. *Evaluation of different regionalization methods*

We employ both regionalized hydrological models, KNN, both statistical approaches and the benchmark method (median hydrological model parameter set across all catchments) to simulate Qmed, Q50 and Q95 for all 44 catchments. Results are then compared with observations to evaluate each approach using the RE criterion (Eq. 10) (see Fig. 5). The best (minimum RMSE) *K* in the KNN method for simulation of Q50, Q95 and Qmed was found to be 5, 9 and 2, respectively. For Q50 all methods, even the simple benchmark, performed similarly. However, regionalized GR4J_MLR method and GR6J_NL show slightly better performance (Fig. 5a). For simulating Q95 the GR6J_RF performs the best. Notably, GR6J_MLR and GR6J_NL result in a wide spread in RE values across catchments, indicating the sensitivity of results to the method taken to regionalize the model parameters. For Q95 large underestimates are associated with the simple benchmark method and the statistical approach based on directly using catchment descriptors. While the KNN method has a comparable median RE across catchments to GR6J_RF, the spread of RE values across catchments is considerable (Fig. 5b). For Qmed, the KNN and statistical method show the best median RE scores, however the spread of values across catchments is considerable for both, indicating poor performance for some catchments. GR4J_MLR and GR4J_RF show modest positive bias,

Table 1
Selected predictors for GR4J parameters based on different objective functions and regionalization methods.

Target	Objective Functions	Target (Predictant)	Regionalization method	Selected predictors	Correlation coefficient
High-flow simulation (Qmed)	NSE-RE (Qmed)	X1	MLR	FARL + ALLUV + FAI + BFIsoil	0.444
			NL	FARL + ALLUV + BFIsoil + FLATWET + SAAPE + DRAIND + FAI	
		X2	MLR	FARL + FOREST + ARTDRAIN2+Temperature	0.484
			NL	FARL + ALLUV + BFIsoil + FLATWET + SAAPE + DRAIND + FAI + FOREST + ARTDRAIN2+DRAIND + Temperature	
		X3	MLR	FARL + BFIsoil + STMFRQ + Temperature	0.692
			NL	FARL + TAYSLO + BFIsoil + AREA + FAI + S1085+ARTDRAIN2+Mean_elevation + DRAIND	
		X4	MLR	AREA + FARL + Elevation_range	0.514
			NL	FARL + Mean_elevation + TAYSLO + S1085+MSL + NETLEN + ARTDRAIN + Elevation_range + ALLUV + FAI	
Low-flow simulation (Q95)	logNSE-RE (Q95)	X1	MLR	FLATWET + SAAPE + BFIsoil + DRAIND	0.352
			NL	DRAIND + SAAPE + FLATWET + Mean_elevation + ALLUV + FARL + BFIsoil	
		X2	MLR	FARL + PEAT + MSL + Elevation_range + Temperature	0.478
			NL	STMFRQ + ALLUV + BFIsoil + FLATWET + SAAPE + DRAIND + SAAR + FOREST + ARTDRAIN2+DRAIND + Temperature	
		X3	MLR	BFIsoil + Elevation_range	0.692
			NL	Elevation_range + SAAPE + FAI + BFIsoil + S1085+STMFRQ + AREA + FARL + PEAT	
		X4	MLR	FARL + DRAIND	0.578
			NL	FARL + TAYSLO + MSL + Mean_elevation + Elevation_range + NETLEN + DRAIND + FAI + AREA + S1085	
Average flow (Q50)	npKGE-RE (Q50)	X1	MLR	ALLUV + DRAIND	0.315
			NL	FARL + ALLUV + BFIsoil + FLATWET + SAAPE + DRAIND + FAI	
		X2	MLR	SAAR + PEAT + ARTDRAIN2+Mean_elevation + Temperature	0.528
			NL	Temperature + DRAIND + BFIsoil + SAAPE + ALLUV + FARL + AREA + NETLEN + FLATWET + PEAT + FARL	
		X3	MLR	ALLUV + BFIsoil + STMFRQ + Temperature	0.692
			NL	FARL + FOREST + SAAR + ALLUV + BFIsoil + MSL + S1085+NETLEN + STMFRQ	
		X4	MLR	FARL + PEAT + Mean_elevation	0.634
			NL	Mean_elevation + FARL + Elevation_range + TAYSLO + MSL + AREA + S1085+STMFRQ	

systematically underestimating Qmed, however the spread of results across catchments is more stable (Fig. 5c). While both optimized GR4J and GR6J performed similarly well in simulating flow metrics using NSGA-II multi-objective optimization algorithm (Figs. S2 and S3), they perform differently when regionalized for simulating different components of the flow regime. While both GR4J and GR6J, when regionalized, underestimate Qmed, GR4J_MLR and/or GR4J_RF are preferred candidate for regionalization of high flows, while GR6J_RF performed better for low flows.

3.4. Spatial distribution of relative error (RE)

The spatial distribution of RE in simulating Q50, Q95 and Qmed across catchments using the GR4J and GR6J models regionalized using MLR, NL and RF methods are illustrated in Figs. 6–8. The same maps for Benchmark, KNN and Statistical methods are depicted in Figs. S4-S6. Evident is the fact that different regionalization methods perform differently across catchments. GR4J_MLR and GR4J_NL perform satisfactorily across most catchments in simulating Q50 (Fig. 6). Also, our simple benchmark method resulted in acceptable outputs for Q50 over most catchments (Fig. S4). Q95 shows the largest spread in RE values across catchments in comparison to Q50 and Qmed.. The GR4J model regionalized with all methods tends to underestimate low flows in eastern, midland and southwest regions. GR6J_RF shows better performance over most catchments (Fig. 7). With the exception of KNN, other methods, i.e. statistical and benchmark, underestimate low-flows over most catchments (Figure S5), however KNN shows a large spread in performance across catchments. Finally, while both models tend to underestimate Qmed, GR4J_MLR and GR4J_RF outperform the other models/methods over most catchments in simulating Qmed (Fig. 8). The benchmark method tends to overestimate Qmed for most catchments and the statistical method over mid-land catchments. For high-flows, KNN seems to be a more robust method compared to benchmark and | statistical methods, but the range of RE values across catchments remains large (Fig. S6).

3.5. Relationship of error with catchment characteristics

To further examine the performance of regionalization methods we correlate the RE for each method with available Physical Catchment Descriptors (PCDs) (Fig. 9). For Q50, RE from the statistical method shows the largest number of significant correlations

Table 2
As Table 1 but for GR6J.

Target	Objective Functions	Target (Predictant)	Regionalization method	Selected predictors	Correlation coefficient
High-flow simulation (Qmed)	NSE-RE (Qmed)	X1	MLR	FARL + FOREST + NETLEN + S1085	0.328
			NL	DRAIND + S1085+SAAR + ALLUV + FLATWET + SAAPE + ARTDRAIN + MSL + Elevation_range	
		X2	MLR	Temperature	0.383
			NL	FARL + MSL + TAYSLO + FLATWET + SAAPE + S1085+SAAR + FOREST + AREA + DRAIND + Temperature	
		X3	MLR	FLATWET + BFIsoil + NETLEN	0.627
			NL	STMFRQ + S1085+BFIsoil + TAYSLO + NETLEN + Mean_elevation + AREA + PEAT + MSL	
		X4	MLR	FARL + FLATWET + BFIsoil + DRAIND + Mean_elevation	0.607
			NL	TAYSLO + FARL + Mean_elevation + Elevation_range + MSL + ARTDRAIN + AREA + FOREST + NETLEN + FAI + S1085	
		X5		PEAT + FLATWET + BFIsoil + DRAIND + Temperatue	0.318
				BFIsoil + SAAR + FLATWET + S1085+STMFRQ + AREA + PEAT + TAYSLO + ARTDRAIN + DRAIND + Mean_elevation	
		X6	MLR	FAI + DRAIND + ARTDRAIN	0.205
			NL	NETLEN + STMFRQ + TAYSLO + SAAPE + BFIsoil + S1085+AREA + FARL + ARTDRAIN2+ARTDRAIN	
Low-flow simulation (Q95)	logNSE-RE (Q95)	X1	MLR	FARL + BFIsoil	0.325
			NL	FARL + ALLUV + BFIsoil + FLATWET + SAAPE + DRAIND + FAI + S1085+SAAR + PEAT	
		X2	MLR	BFIsoil + DRAIND + TAYSLO + Elevation_range	0.48
			NL	FARL + ALLUV + BFIsoil + FLATWET + SAAPE + DRAIND + FAI + FOREST + ARTDRAIN2+Temperature	
		X3	MLR	MSL + STMFRQ	0.47
			NL	SAAR + TAYSLO + NETLEN + BFIsoil + DRAIND + MSL + AREA + S1085+ARTDRAIN	
		X4	MLR	FARL + FLATWET + BFIsoil + S1085+Mean_elevation	0.655
			NL	FARL + MSL + Mean_elevation + TAYSLO + S1085+Elevation_range + NETLEN + AREA + ARTDRAIN + DRAIND+ FOREST	
		X5	MLR	SAAR + FLATWET + Elevation_range + Temperature	0.321
			NL	BFIsoil + DRAIND + FAI + Elevation_range + FARL + NETLEN + S1085+MSL + SAAPE + TAYSLO + FARL	
		X6	MLR	FAI + BFIsoil + TAYSLO + Mean_elevation + Temperature	0.492
			NL	FLATWET + Elevation_range + BFIsoil + PEAT + SAAPE + SAAR + S1085+ARTDRAIN + TAYSLO + DRAIND + FARL	
Average flow (Q50)	npKGE-RE (Q50)	X1	MLR	DRAIND	0.435
			NL	DRAIND + SAAR + BFIsoil + FOREST + ALLUV + SAAPE + Mean_elevation + FAI + Elevation_range	
		X2	MLR	SAAR + TAYSLO + Mean_elevation + Temperaure	0.596
			NL	FARL + ALLUV + BFIsoil + PEAT + SAAPE + AREA + FAI + NETLEN + FLATWET + DRAIND + Temperature	
		X3	MLR	SAAR + BFIsoil + Temperature	0.47
			NL	BFIsoil + MSL + SAAR + TAYSLO + S1085+ALLUV + FARL + Temperature + DRAIND	
		X4	MLR	FARL + PEAT + BFIsoil + Mean_elevation	0.643
			NL	FARL + TAYSLO + Mean_elevation + Elevation_range + MSL + AREA + PEAT + NETLEN + SAAR + S1085+ALLUV	
		X5	MLR	SAAR + ALLUV + NETLEN + TAYSLO + Elevation_range	0.292
			NL	SAAR + ALLUV + FOREST + FARL + MSL + FAI + ARTDRAIN2+FLATWET + BFIsoil + Mean_elevation + NETLEN	
		X6	MLR	SAAR + ALLUV + FAI + NETLEN + Elevation_range	0.337
			NL	FAI + TAYSLO + SAAPE + ARTDRAIN + Elevation_range + DRAIND + ARTDRAIN2+Mean_elevation + BFIsoil + PEAT +FARL	

(0.05 level) with PCDs, followed by benchmark application of the hydrological models. Largest positive correlations are shown for PCDs that relate to catchment wetness, including SAAR, the proportion of peat in the catchment (PEAT) and wetness of soils (FLATWET). For Q50 KNN, GR6J_MLR and GR4J_NL show the fewest significant correlations between RE and PCDs. For KNN and GR6J_MLR, RE is significantly negatively correlated with the presence of reservoirs and lakes (FARL) and higher levels of potential evapotranspiration (SAAPE) and significantly positively correlated with FLATWET. GR4J_NL RE shows significant positive correlations with groundwater storage (BFIsoil) and temperature and significant negative correlations with drainage density (DRAIND) and mean catchment elevation.

Table 3
Performance of regionalization methods in predicting GR4J and GR6J parameters.

	OFs	Parameter	R^2			RMSE		
			MLR	NL	RF	MLR	NL	RF
GR4J model	npKGE-RE(Q50)	X1 (mm)	0.26	0.29	0.77	113.2	110.8	79.71
		X2 (mm/day)	0.48	0.28	0.36	0.65	0.76	0.89
		X3 (mm)	0.59	0.31	0.78	83.3	107.74	78.02
		X4 (day)	0.54	0.69	0.81	0.41	0.34	0.32
	LogNSE-RE(Q95)	X1 (mm)	0.34	0.27	0.84	155.46	162.45	112.13
		X2 (mm/day)	0.53	0.33	0.81	0.86	1.02	0.69
		X3 (mm)	0.35	0.39	0.75	115.43	112.14	89.66
		X4 (day)	0.56	0.57	0.76	0.42	0.41	0.36
	NSE-RE(Qmed)	X1 (mm)	0.42	0.35	0.8	112.25	118.35	92.62
		X2 (mm/day)	0.48	0.33	0.69	1.33	1.52	1.33
		X3 (mm)	0.7	0.57	0.83	78.1	92.88	72.38
		X4 (day)	0.51	0.37	0.75	0.4	0.45	0.33
GR6J model	npKGE-RE(Q50)	X1 (mm)	0.3	0.34	0.71	64.28	62.15	45.75
		X2 (mm/day)	0.4	0.14	0.05	0.37	0.44	0.59
		X3 (mm)	0.45	0.37	0.76	89.67	95.55	77.61
		X4 (day)	0.63	0.47	0.85	0.37	0.44	0.29
		X5 (-)	0.33	0.25	0.8	0.33	0.35	0.25
		X6 (mm)	0.51	0.29	0.74	9.39	11.34	8.7
	LogNSE-RE(Q95)	X1 (mm)	0.28	0.35	0.72	90.44	85.76	65.14
		X2 (mm/day)	0.48	0.39	0.67	0.28	0.31	0.26
		X3 (mm)	0.18	0.25	0.7	60.8	58.05	44.67
		X4 (day)	0.64	0.5	0.8	0.37	0.43	0.32
		X5 (-)	0.29	0.26	0.75	0.29	0.29	0.22
		X6 (mm)	0.28	0.29	0.78	12.17	12.09	9.67
	NSE-RE(Qmed)	X1 (mm)	0.34	0.26	0.77	55.81	58.95	43.16
		X2 (mm/day)	0.27	0.31	0.3	0.73	0.71	1
		X3 (mm)	0.64	0.45	0.82	77.55	95.48	59.82
		X4 (day)	0.61	0.39	0.77	0.38	0.48	0.34
		X5 (-)	0.32	0.31	0.8	0.24	0.24	0.18
		X6 (mm)	0.21	0.24	0.63	17.49	17.2	14.94

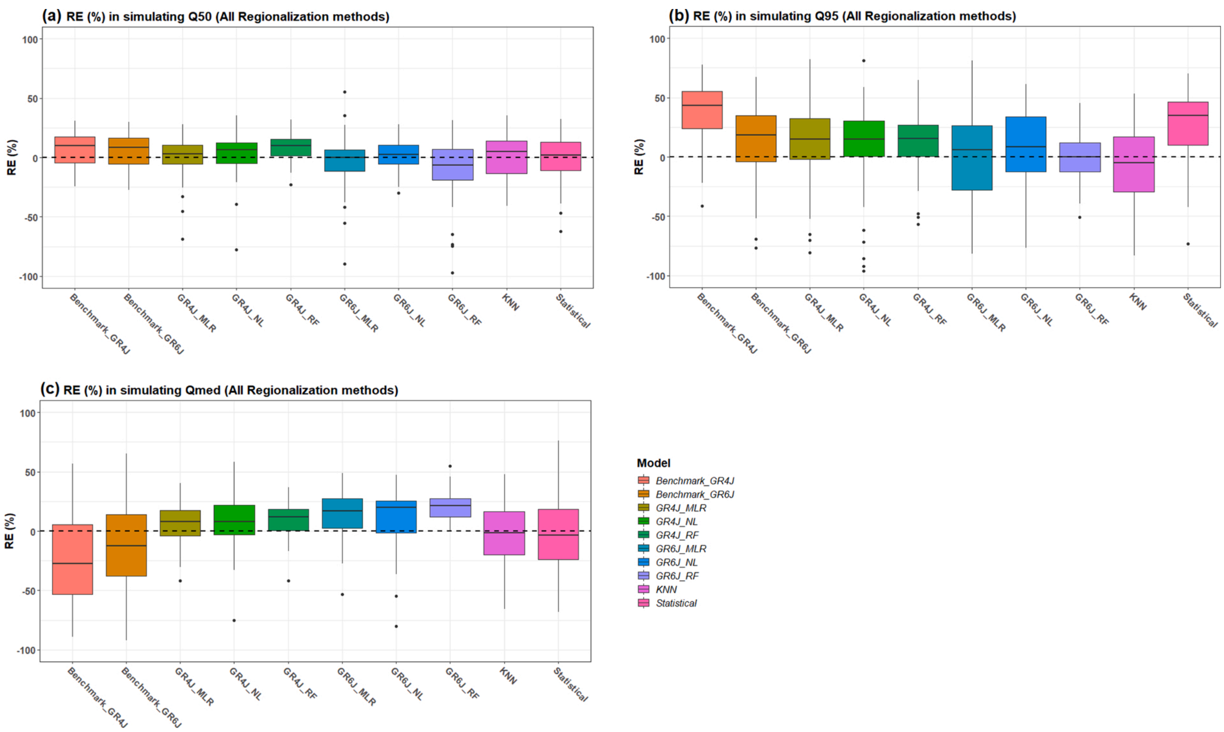

Fig. 5. Relative Error (RE %) of different regionalization methods in simulating a) Q50 b) Q95 and c) Qmed across the study catchments. Positive RE indicated underestimation and negative RE overestimation.

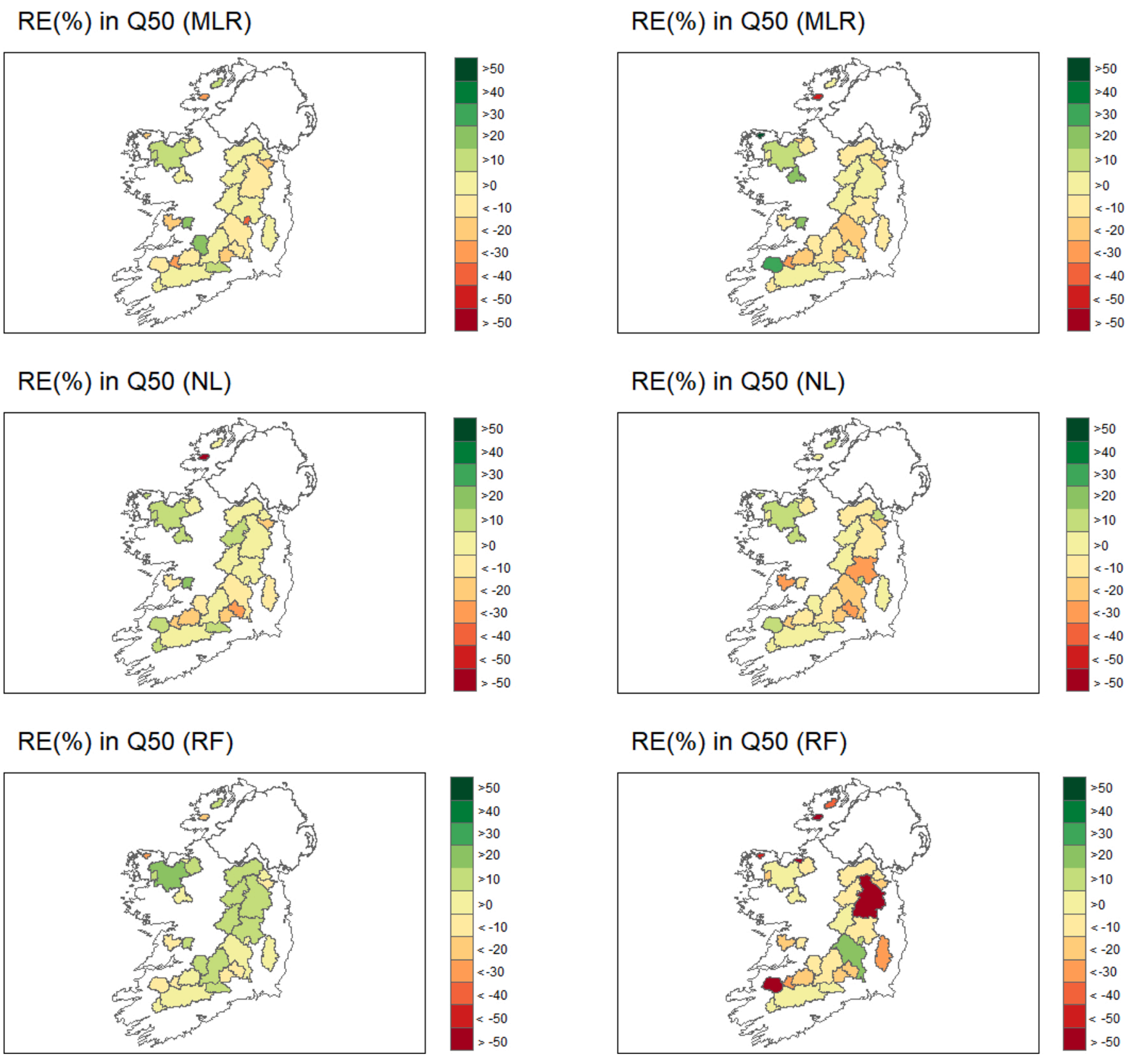

Fig. 6. Relative Error (RE %) distribution in simulating Q50 over study catchments using regionalized parameters of GR4J (left column) and GR6J (right column) using MLR, NL and RF methods.

Correlation analysis of Q95 RE with PCDs reveals the largest numbers of significant correlations for benchmark and statistical methods. The fewest significant correlations between RE and PCDs are evident for KNN, followed by GR4J_RF and GR6J_RF. RE for KNN shows no significant correlations with available PCDs, while GR4J_RF shows only one significant positive correlation with elevation range within the catchment. GR6J_RF shows significant positive correlations with the Flood Attenuation Index (FAI), groundwater storage (BFIsoil) and PCDs related to the presence of arterial drainage in the catchment. RE for GR6J_RF also shows significant negative correlation with mean elevation.

For Qmed RE, the greatest number of significant correlations with PCDs are evident for the benchmark and statistical method. The fewest significant correlations are evident for GR4J_RF and GR4J_NL. For the former, RE shows a significant positive correlation with the presence of reservoirs and lakes (FARL) and arterial drainage, while a significant negative correlation is evident for Qmed RE with elevation range. GR4J_NL shows significant negative correlations with FAI, network length (NETLEN), steam frequency (STMFRQ) and temperature.

4. Discussion

This paper has examined the potential to regionalize hydrological models for prediction in ungauged catchments in Ireland. In doing so we focused attention on high, medium and low flows, the evaluation of different methods for regionalizing model parameters, while benchmarking the performance of regionalized models (in terms of RE), against available statistical methods and a simple benchmark using the median parameter set across all catchments. In the majority of cases regionalization of hydrological model parameters improved performance over available statistical and benchmark methods, however notable differences in performance are

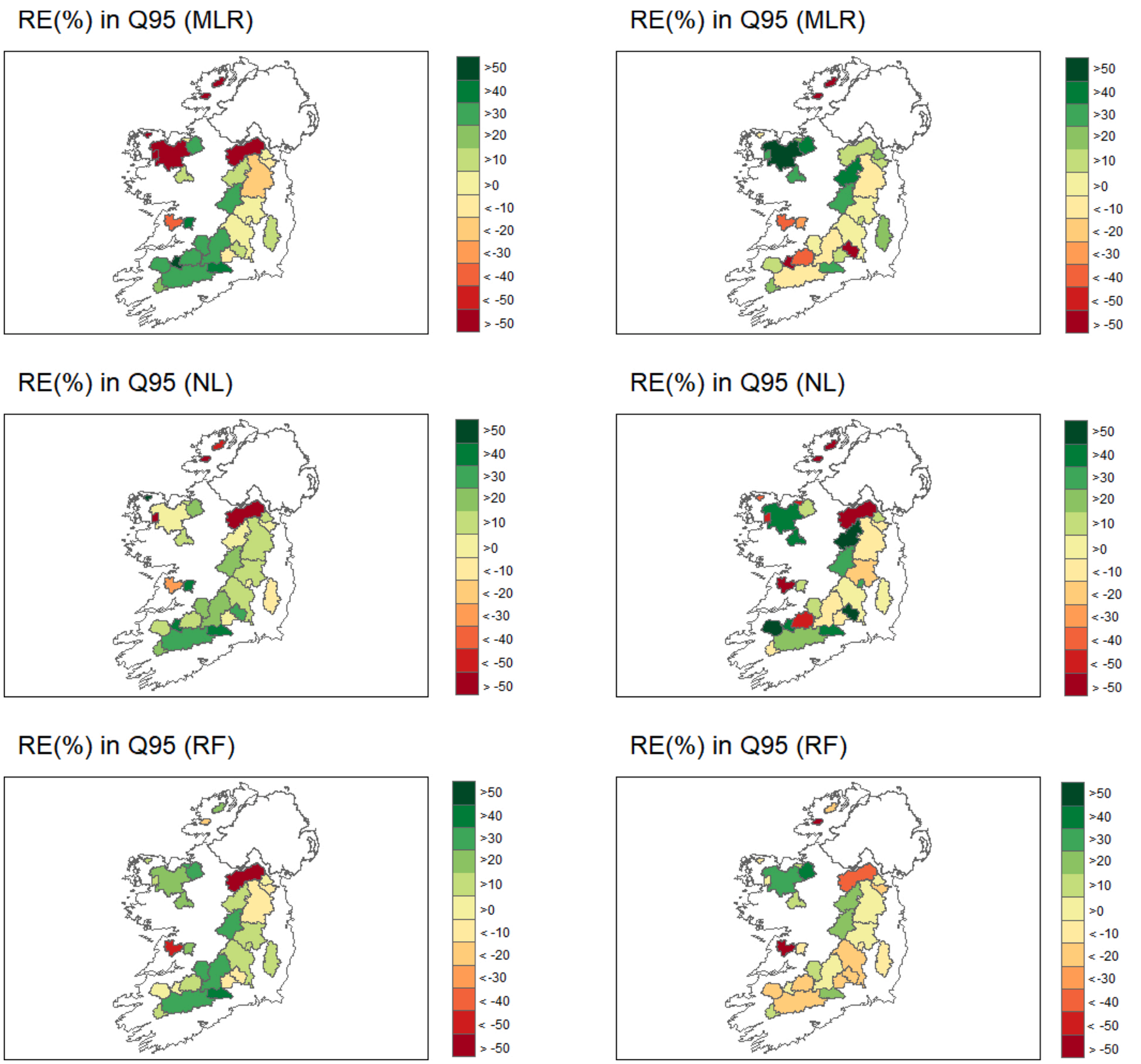

Fig. 7. As Fig. 6 but for low flows (Q95).

evident depending on the model used and the component of the flow regime of interest.

Regionalisation was least satisfactory for low flows, with largest spread in RE estimates across the catchment sample in comparison with median and high flows. Regionalization of the GR6J model was more successful in predicting Q95, relative to GR4J which tended to produce large underestimates, indicating the importance of the non-linear baseflow processes involved in low flow response. Other studies by Pushpalatha et al. (2011); Pushpalatha (2013) and Sadegh et al. (2019) also found that considering additional storage by introducing a groundwater exchange threshold (X5) and additional routing store (X6) to the GR4J model can improve simulation of low-flow conditions in catchments where groundwater has a greater contribution to discharge. Regionalization of GR6J parameters using MLR and NL did not result in better outcomes relative to the simple benchmark method of using the median parameter set derived from all catchments. Only the application of random forests resulted in improvement. The RF method provided the best results in capturing the optimized values for the additional groundwater parameters in the GR6J model (X5 and X6) and was able to incorporate the information content from all available PCDs. Considerably poorer results for these parameters were returned for MLR and NL methods, despite the complexity of the latter in terms of number of PCDs included.

While the GR6J_RF regionalization provided the best median RE scores for Q95 across the catchment sample, there was still considerable spread in RE values, making it difficult to recommend it in all cases. Significant positive correlations between Q95 RE and BFIsoils, indicates a tendency towards underestimation of Q95 in catchments where groundwater storage is greatest. Despite the additional groundwater parameters in the GR6J model, baseflow contributions in the regionalized model may be underestimated. GR6J_RF also tends to underestimate Q95 for catchments influenced by reservoirs and lakes (FARL) and those affected by arterial

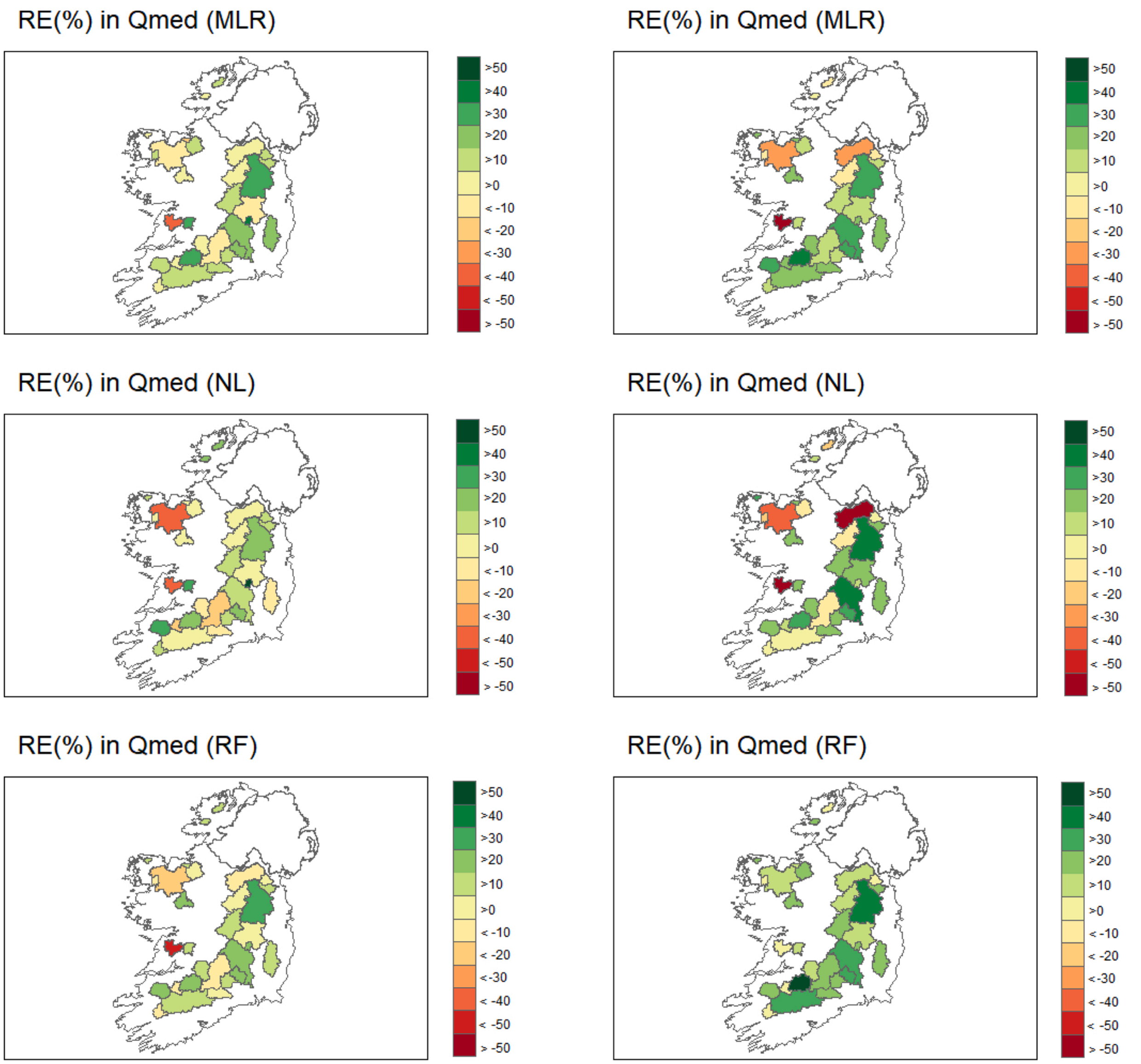

Fig. 8. As Fig. 6 but for high flows (Qmed).

drainage; a process of agricultural land improvement and channel straightening and dredging undertaken in Ireland (Bree and Cunnane, 1979). Future work should investigate the potential to regionalize a more complex hydrological model that might better represent flow paths in the highly permeable catchments and the impacts of arterial drainage on catchment response (e.g. SMART model (Mockler et al., 2016)). The impact of arterial drainage on low flows in Ireland has not been widely studied. The relative error associated with regionalization found here would indicate that arterial drainage may artificially increase low flows.

In relation to high flows, both regionalized models tend to underestimate Qmed (positive median RE), however underestimates tend to be greater for GR6J. Qmed prediction was also less sensitive to regionalization method, perhaps due to the more linear rainfall runoff response at high flows. Both GR4J_MLR and GR4J_RF produced similar median RE scores, however the spread of RE values across the catchment sample was more constrained using random forests, again indicating its ability to better generalize across the sample. Regionalisation using random forests also resulted in fewer significant correlations between RE and PCDs. However, significant correlations were found with FARL and arterial drainage, indicating that the presence of both is associated with larger underestimates of Qmed. The impact of arterial drainage on high flows in Ireland has been well documented (e.g. Harrigan et al., 2014). Interestingly, the statical methods evaluated resulted in better estimates of median RE for Qmed, however, performance was more variable across the catchment sample.

It has been shown by many researchers (e.g. Yapo et al., 1998) that single objective function methods in calibrating conceptual hydrological models may lead to optimized models which fail to properly represent/simulate important characteristics of observed flow. In calibrating both GR4J and GR6J we show that multi-objective optimization improves the performance of models compared to

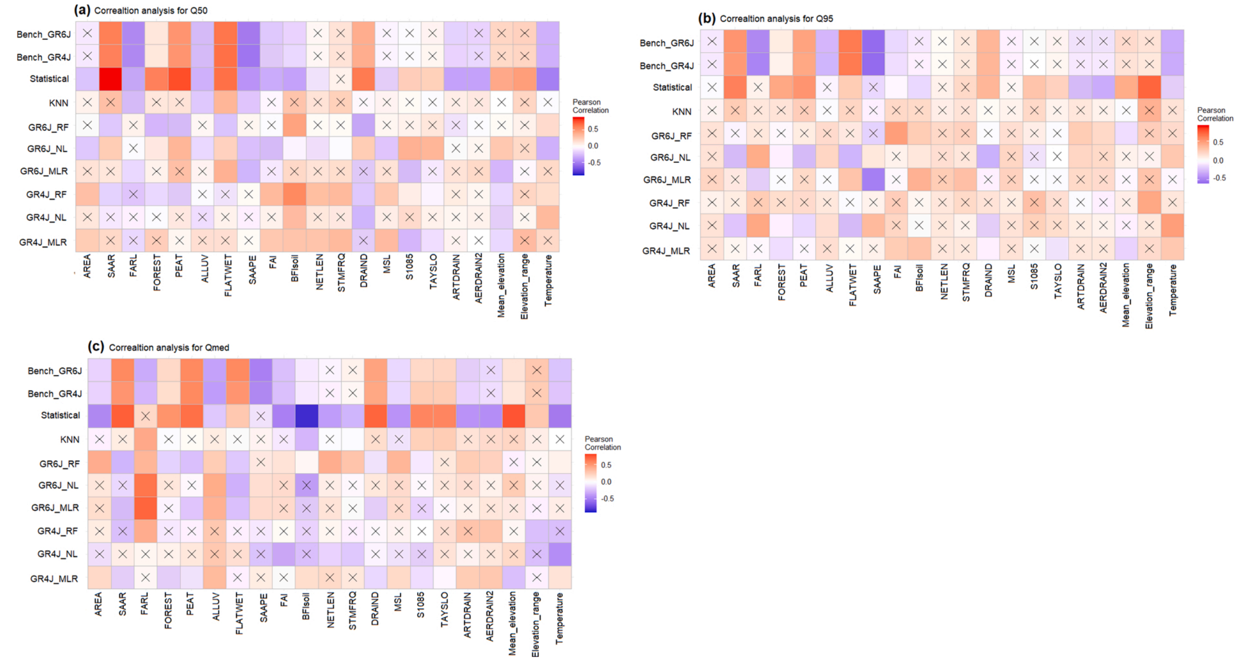

Fig. 9. Heatmap of correlation values between Physical Catchment Descriptors (PCDs) and RE(%) for different regionalization methods for simulation of a) Q50 b) Q95 and c) Qmed (note that *non-significant* correlation values at 5% significance level are marked by a cross).

the uni-objective function case. It has also been shown in previous studies that the equifinality problem can be reduced when hydrologic models are calibrated using a multi-objective framework (Ruelland et al., 2010). We also show the importance of selecting suitable objective functions in simulating high and low flow regimes which has also been shown by other researchers e.g. Garcia et al. (2017); Kim et al. (2018).

Overall, there is no universal approach that performs best for all catchments and different parts of the flow regime, highlighting the need for regionalization study design to focus on the component of the flow regime of interest. Diversity in catchment physical characteristics and climatic variability can lead to different performances for application of each regionalization method over various regions (Razavi and Coulibaly, 2013). Clark et al. (2017) suggest that regionalization of hydrologic model parameters using regression methods are more accurate in flow simulation compared to simpler regionalization methods such as spatial proximity and similarity-based approaches. While MLR has been widely applied to regionalize parameters of hydrological models at ungauged basins, we show that the method applied to regionalize model parameters can have a significant influence on the results. Other researchers have found similar results, indicating that identification of a single best model is very difficult for all catchments and criteria, especially for low-flow simulations (e.g. Nicolle et al., 2014), which are often heavily dependent on catchment characteristics (Razavi and Coulibaly, 2013). We find that the use of the random forest method offers a powerful method to generalize the relationship between catchment descriptors and model parameters, relative to linear and non-linear regression.

Finally, this work represents a first formal attempt at regionalizing hydrological models for Irish catchments and adds to the toolkit available for simulating flows in ungauged catchments. Importantly, the ability to produce continuous simulations at ungauged catchments widens the type of hydrological analysis that can be undertaken for ungauged catchments. However, there are limitations to the work undertaken. Results are dependent on our catchment sample and the physical catchment descriptors used to estimate optimized model parameters. Future work should aim to diversify the set of catchment descriptors used and to include catchments that are under-represented, e.g. smaller catchments in coastal locations. We chose the GR4J and GR6J models due to their parsimonious nature, requiring only four and six parameters to be calibrated, respectively. Given the challenges in simulating low flows in particular, future work should also attempt to regionalize other hydrological models for Irish catchments and explore the added value of other machine learning techniques for regionalizing model parameters. Lastly, future work should further assess the parameter uncertainties associated with regionalization of conceptual models in ungauged catchment (Estacio et al., 2021).

5. Conclusion

We regionalize two hydrological models (GR4J and GR6J) for continuous simulation of discharge in ungauged catchments using 44 Irish catchments. Using different approaches (multiple linear regression, non-linear regression and random forests) we find that random forests outperform traditional methods for linking model parameters with physical catchment descriptors. By comparing performance with other approaches to regionalize low, medium and high flows (K nearest neighbors (KNN), regression on physical descriptors), we find that our regionalized models compare favorably in terms of relative error. While all regionalization approaches, including a simple benchmark of using median parameter sets from across all catchments to run hydrological models, perform well for average flow conditions (Q50), we find that random forests offer the best potential to generalize across catchments, resulting in best median RE scores and reduced spread in RE across the catchment sample. The GR4J(GR6J) model regionalized using random forests perform best for simulating high flows (Qmed) and low flows (Q95), respectively. Our results highlight that the objectives for regionalizing hydrological models are critical to the selection of methods. While the simulation of average flow conditions was less sensitive, the choice of hydrological model, objective functions for optimization and approach for linking model parameters and physical catchment descriptors had a large influence on the success of regionalization for high and low flows.

Author statements

Saeed Golian was responsible for developing the ideas, designing the methodology, developing the required codes, data analyses and visualization and finally writing the manuscript.

Conor Murphy contributed in developing the ideas, developing the methodology, checking for research outputs and finally writing and revising the manuscript.

Hadush Meresa helped in designing a part of methodology, running some codes for random forest and nonlinear methods, and finally revising the manuscript.

Declaration of Competing Interest

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

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.ejrh.2021.100859.

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