

Persistent neural calibration for discharges modelling in drought-stressed catchments

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ABSTRACT

Cross-sector coordination between all water uses and the environmental flows is an essential target for achieving sustainable management in any hydrographic region. In this framework, a novel neural approach was developed and implemented, by the software ANNPI 1.0, to characterise and infer of the discharges regime in a specific basin using only a few attributes as independent variables. The calibration procedure is controlled by the Persistence Index (PI), which is function of a determined estimation lead-time, to facilitate the dynamic character of these simulations. A model validation was carried out in the Lower Guadiana Transboundary Basin, in the Southwest Iberian Peninsula, characterised by moderate and severe drought cyclical events. The best neural approaches included as input variable, between others, the Standardized Precipitation Index at a twelve-month scale SPI(12) that is indicator of hydrological drought, obtaining results statistically very good with determination coefficients higher to 0.77, Nash-Sutcliffe Efficiency coefficients higher to 0.75, Kling-Gupta Efficiency coefficients higher to 0.87 and Persistence Indexes higher to 0.60 in three of the four reservoirs analysed. These accuracy measures showed the ability of the software ANNPI 1.0 to reduce the naïve effect in the forecasting of streamflows time series and could therefore facilitate the development of decision-support systems to make reliable reservoir water balance simulations which will allow to assess future water availability to ensure the main ecosystem services.

1. Introduction

In the water management plans of any hydrographic region, there is a clear need to have a balanced allocation of all water uses —irrigation, urban and industrial supply, hydropower production, recreation— and their compatibility with the ecological flows to achieve the three dimensions of sustainable development: social, economic, and environmental (ONU, 2015; Li et al., 2023). In order to achieve this priority, it is necessary the seasonal and interannual assessment and characterisation of water resources available in the basin to support future decisions regarding the different water allocations (Cabrera & Babiano, 2007; Omedas et al., 2008; Serrano et al., 2020). For this purpose, the administrations responsible for water management have usually simulated data on inflows in the basins (discharges) that are contrasted and validated with records, in selected locations (strategic water bodies), carried out by means of systems for acquiring real flows.

In this context, the approach, development and implementation of models that can simulate, characterise, infer and estimate with an

acceptable goodness of fit the discharges in the basins to be managed is postulated as a proposal to be highlighted among the priority tasks for integrated water resources planning and, fundamentally, in hydrographic basins located in regions with typical hot-summer Mediterranean climate conditions and characterized by a high seasonal and interannual variability of the precipitation regime (Beck et al., 2018) that sometimes leads to drought events that repeat cyclically. In these drought periods, it can be difficult to ensure a balanced allocation of all water uses and their compatibility with the environmental flows required to sustain aquatic ecosystems and the human well-being that depends on them (García-Ruiz et al., 2011; Arthington, 2012; Garrote et al., 2016; Mehr et al., 2020; Altunkaynak & Jalilzadnezamabad, 2021; Dalcin et al., 2023). Thus, the models to be used should have the versatility to be able to simulate and adapt to the behaviour of the water resources system under various possible hydrological scenarios, in order to allow a dynamic and balanced allocation of the different water uses without putting ecosystems at risk (Global Water Partnership, 2000; Zingraff-Hamed et al., 2018; Pulido-Calvo et al., 2020).

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The simulation and estimation of the dynamical behaviour of the inflows of a basin involves the study and analysis of time sequences of hydro-climatic variables (multivariate time series), with highly non-linear characteristics, which leads to the need for the modelling of interrelated stochastic processes (Raman & Sunilkumar, 1995; Pulido-Calvo et al., 2012; Wang et al., 2023). Generally, available theoretical (or analytical) models, which are based on physical laws that represent and describe the behaviour of the components of a river basin, require diverse and varied calibration parameters, such as characteristics of vegetation and soils, among others, which complicate the modelling procedure of these hydrological processes mainly in those basins where these data are not available or are not easy to obtain (Razavi & Coulibaly, 2013; Beven & Chappell, 2021; Ochoa-Tocachi et al., 2022).

In the last two decades and as a result of advances in computing techniques, empirical (or numerical) methods, which are based on observations of some of the variables significantly involved in the hydrological process, obtained in certain locations and conditions, are being used quite frequently to simulate and predict the dynamics of water resource systems. These data-based methodologies often provide, with a parsimonious predictive model, a better fit than the hydrological models based on process representations because they have the ability to learn time series relationships and spatial relationships in the same predictive framework (Kratzert et al., 2019; He et al., 2023; Yao et al., 2023).

Among this category of data-driven approaches are artificial neural networks. Several studies have shown that an artificial neural network trained using only time-dependent meteorological inputs and, sometimes, some ancillary static catchment attributes, was well suited for the streamflow regional modelling on catchments (Goswami et al., 2007; Besaw et al., 2010; Pulido-Calvo et al., 2012; Kratzert et al., 2018, 2019; Nogueira-Filho et al., 2022; Anh et al., 2023).

Therefore, in this work, the analysis and modelling, by means of Artificial Neural Networks (ANNs), of the discharges natural regime (streamflows) of the hydrographic region of the International Lower Guadiana River, in the province of Huelva (Andalucía) in Spain and the regions of the Baixo Alentejo and Algarve in Portugal – the Lower Guadiana Transboundary Basin – was carried out. This basin of the Southwest Iberian Peninsula has typical conditions of a hot-summer Mediterranean climate with a high hydric stress due to the concurrence of moderate and severe drought seasonal events and a growing demand for water use, mainly for irrigated agriculture that plays a key role in the economic development of the region. In addition, this Algarve-Baixo Alentejo-Andalucía Euroregion comprises natural spaces classified by the Natura 2000 Network by having sites of ecological high importance in Spain and Portugal (European Commission, 2008; Guimarães et al., 2012; Carmona et al., 2013; Moura et al., 2017; Pulido-Calvo et al., 2020).

As a novelty in this research, a modification in the calibration scheme of the standard back-propagation algorithm of ANNs was proposed to reduce the naïve effect that implies estimates similar to the observed data in the previous time period when working with time series (Park, 1998; Abrahart & See, 2000; Gutiérrez-Estrada et al., 2005; Pulido-Calvo & Portela, 2007; Pulido-Calvo & Gutiérrez-Estrada, 2009) and, consequently, to facilitate the simulation and modelling of the dynamical behaviour of streamflows. For this purpose, the ANNPI 1.0 computer application has been designed and programmed, combining a graphical interface developed in Microsoft Visual Basic 6.0, the R package *neuralnet* developed by Fritsch et al. (2016) and a calculation engine for the evaluation of the neural approximations as well as for the automatic control of the variation of the calibration parameters used by *neuralnet* (Supplementary material).

For the evaluation of this neural modelling, the results obtained were compared with the discharges estimated by SIMPA (*Sistema Integrado de Modelación Precipitación-Aportación* – in Spanish–, Integrated System for Rainfall-Runoff Modelling), which is a conceptual and quasi-distributed simulation model of the process of transformation of precipitation into runoff in a natural regime. This SIMPA model, developed

at the ‘Centro de Estudios y Experimentación de Obras Públicas de España’ (CEDEX), has been widely used in hydrological studies providing satisfactory results (Estrela & Quintas, 1996; Estrela et al., 1999; Álvarez et al., 2005; Pérez-Martín et al., 2014; Taguas et al., 2015; CEDEX, 2020).

This way, the objectives of this study were:

- i. To know, to understand and to quantify the attributes that characterise the behaviour of water resources system of the Lower Guadiana Transboundary Basin: meteorological data, water uses and future trends, past drought events, streamflows registered in gauging stations and requirements of environmental flows.
- ii. To demonstrate how the proposed neural approach, using some catchment attributes as independent variables, can characterise and infer the temporary of the streamflow in order to achieve an adaptive and integrative water resources regulation management, thus enabling the balanced allocation of all uses and their compatibility with the environmental flows in this international basin.
- iii. To benchmark the performance of the neural network model against the SIMPA model.

2. Material and methods

2.1. Study area: The Lower Guadiana Transboundary basin

The hydrographic region of the Guadiana River is one of the large basins shared by Spain and Portugal in the Iberian Southwest and is also one of the largest shared river fully within the European Union borders (Do Ó, 2012). The Guadiana basin is divided into 3 sub-basins: the upper Guadiana, the middle Guadiana and the lower Guadiana (Carmona et al., 2013). This study focuses on the lower sub-basin in the Algarve and Baixo-Alentejo regions in Portugal and in the province of Huelva (Andalucía) in Spain. This area is located in the southern border between Portugal and Spain in the Southwestern Iberian Peninsula (Fig. 1). Both countries share this hydrographic region of the Lower Guadiana River where the river becomes the border just 70 km above its mouth.

The drainage area of this sub-basin is approximately 8,272 km², of which 6,002 km² are in the Algarve and Alentejo regions in Portugal and 2,270 km² in the province of Huelva (Andalucía) in Spain. The climatic data show a significant spatial and temporal variability in precipitation and temperature registered values. Most precipitation events occur from October to April with annual mean value of 521 mm varying from 264 mm in the low estuary and 1397 mm in the high zones of the catchment. The summer period is characterised by the absence of precipitation. The mean annual temperature is of 18.24 °C with minimum and maximum values that can be of –4 °C in winter and 44 °C in summer, respectively (Pulido-Calvo et al., 2020, 2021).

An analysis and evaluation of hydrological drought events using the Standardized Precipitation Index (SPI), developed by McKee et al. (1993), was made for this hydrographic region of the International Lower Guadiana River. A detailed description of these calculations can be found in the work of Pulido-Calvo et al. (2020). A SPI(12) (12-month time scale) was calculated from 1900 to 2017 using the monthly precipitation series of several climatic stations distributed through this study area. A 12-month SPI is a comparison of the precipitation for 12 consecutive months with that recorded in the same 12 consecutive months in all previous years of available data. Drought episodes occur when the SPI is continuously negative and with a value of –1.0 or lower (SPI from –1.0 to –1.49 indicates moderately dry, from –1.5 to –1.99 severely dry, from –2 and less extremely dry) (WMO, 2012; Eslamian & Eslamian, 2017).

Pulido-Calvo et al. (2020) identified, with the analysis of SPI(12) time series, the rotation of long cycles (25–30 years) with predominance of moderate and severe drought events (from 1920 to 1950 and from

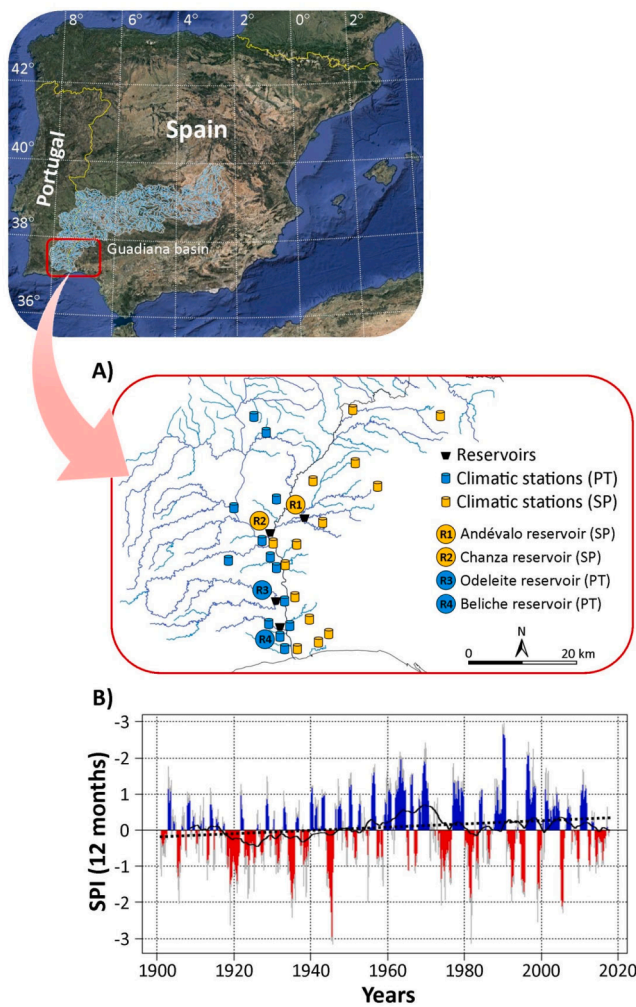


Fig. 1. Hydrographic region of the Guadiana River in the Iberian Peninsula. The red box marks the Lower Guadiana sub-basin: A) Regulating reservoirs and climate stations distributed in all the study area; and B) Standardised Precipitation Index for a time scale of 12 months SPI(12). The linear trend fit of SPI (12) is shown with the dashed line and the 10-year moving average of SPI(12) is shown with the continuous line (modified from Pulido-Calvo et al., 2020). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

1975 to 2005) with precipitation normal regime cycles without episodes of hydrological drought (from 1900 to 1920 and from 1950 to 1970) (Fig. 1). Consequently this implies a high inter-annual and seasonal variability in the discharges regime with intermittent fluvial courses with periods without flows rates. This is also shown in the water volumes variability of the regulating reservoirs (Chanza, Andévalo, Beliche and Odeleite with capacities of 341 hm³, 634 hm³, 48 hm³ and 130 hm³, respectively) which comprise the water resources system in study (Fig. 1). Thus this characterisation of the drought temporal variability, with long-term precipitation patterns, which are tied to streamflows, reflects the importance of considering/representing the SPI(12), which is an proxy indicator of hydrological drought for medium-long-term impacts (European Commission, 2021), to simulate/estimate the dynamics of the Lower Guadiana Transboundary Basin Water System.

The total water demand in this basin is divided as follows: 78 % for irrigated agriculture, 17 % for urban use and 5 % for industrial use. Over the last decades, there has been an increasing trend in the average demand for irrigation water in both the Spanish and Portuguese areas (Fig. 2) (Pulido-Calvo et al., 2021). In recent years, this expansion of the area irrigated is usual in watersheds of southern Iberian Peninsula

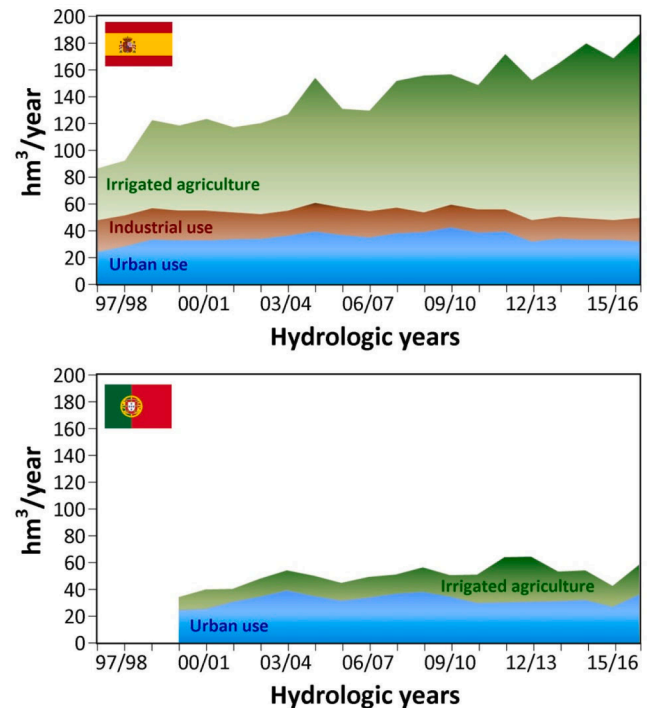


Fig. 2. Evolution of water uses supplied from the Chanza-Andévalo regulating system (Spain) and from the Odeleite-Beliche regulating system (Portugal).

which, in addition, according to the climate change predictions, could be affected by a reduction in available water resources (Iglesias et al., 2005; Rodríguez-Díaz et al., 2007; Pulido-Calvo et al., 2012; Molist, 2023). Additionally Pulido-Calvo et al. (2020) showed by a frequency analysis that the requirements of the environmental flows identified in the Spanish and Portuguese Hydrological Plans (PHDHG, 2016; PGRHG, 2016) were not met in months of years characterised by severe drought events [SPI(12) < -1.5].

2.2. Software ANNPI 1.0: Dynamical simulation of discharges

The simulation of the inflows to the regulation reservoirs of the Lower Guadiana Sub-basin was carried out using Artificial Neural Networks (ANNs). ANNs are mathematical models inspired by the neural architecture of biological nervous systems. The most widely studied and most basic structures are multilayer perceptrons (Rumelhart et al., 1986). These models learn iteratively by introducing an input (independent variables) and output (dependent variable) variables set as many times as necessary until a certain level of error is reached during the calibration phase of the model (an iteration where the whole set of calibration data is introduced to the ANN is called an epoch). Such supervised approaches allow the analysis of complex data sets and the evaluation of non-linear relationships between variables. A detailed description of how multilayer perceptrons work can be found in Hsu et al. (1995), Tsoukalas and Uhrig (1997), ASCE (2000a,b), Shrestha et al. (2005) and Pulido-Calvo and Portela (2007).

A typical three- or four-layer multilayer perceptron has an input layer, one or two hidden layers and an output layer. The processing elements in each layer are called nodes or neurons. An ANN with k , m , n and s nodes in the input, first and second hidden and output layers, first and second hidden and output layers, respectively, has the notation (k, m, n, s) (Fig. 3). The parameters associated with each of the connections between nodes in each layer are called weights (W_{ji}). There are many methods for calibrating or learning neural approaches. In this work, the standard back-propagation algorithm was used.

The standard back-propagation algorithm is based on the error

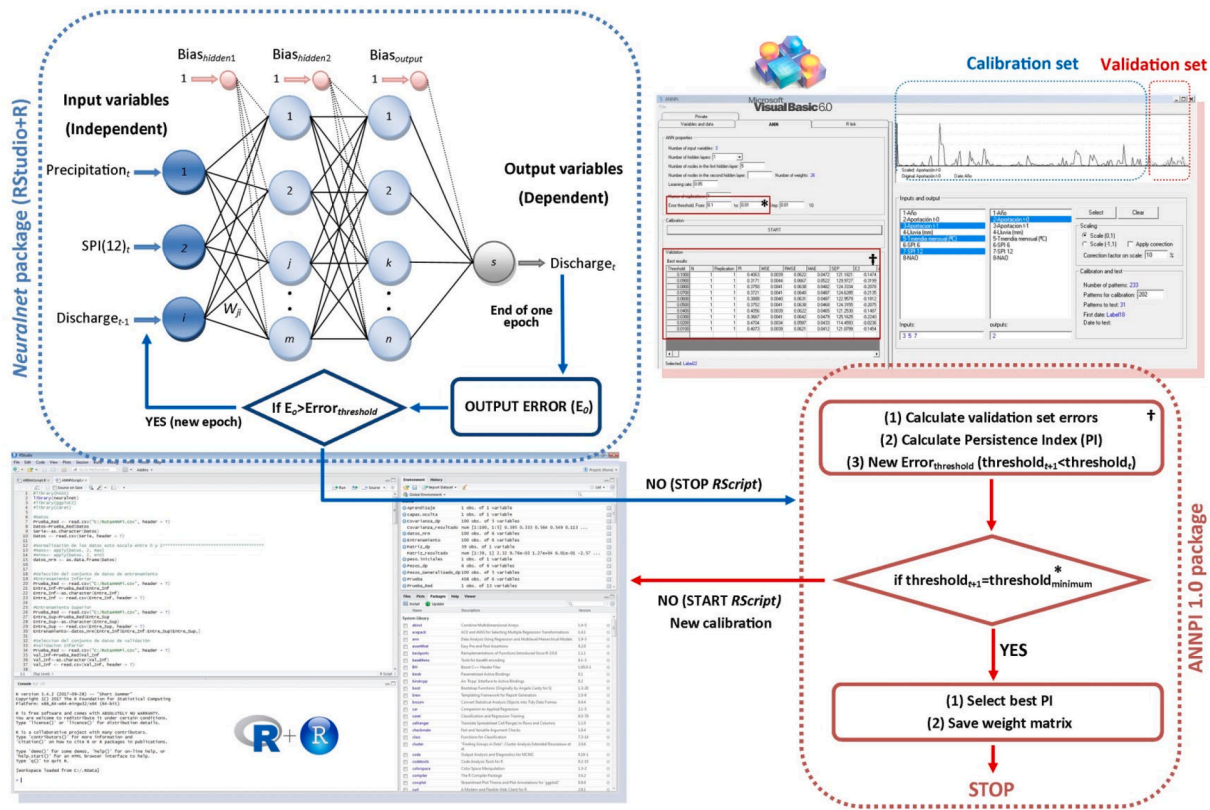


Fig. 3. Flowchart of the ANNPI 1.0 software which integrates a graphical interface developed in Microsoft Visual Basic 6.0 with an independent calculation engine implemented in R 3.4.0. The ANN calibration is carried out using the R package *neuralnet* (Fritsch et al., 2016).

propagation from the output layer to the connections between the output layer and the hidden layer(s) and from the first hidden layer to the input layer. This procedure is repeated after the presentation of each set of calibration values over an epoch, which gives a static character to this neural structure. This results in a tendency to provide simplistic results when working with time series (naïve behaviour), meaning that the estimation provided by the ANN in each time period is systematically very close to the data observed in the previous time period. This behaviour has been described in a multitude of papers analysing time series of very different nature (Park, 1998; Abrahart & See, 2000; Gutiérrez-Estrada et al., 2005; Pulido-Calvo & Portela, 2007; Pulido-Calvo & Gutiérrez-Estrada, 2009). On the other hand, naïve behaviour is favoured by significant autocorrelation and cross-correlation of the variables, so it is extremely important the selection of appropriate inputs to the ANN models (Bowden et al., 2005; May et al., 2008; Fernando et al., 2009; Gutiérrez-Estrada et al., 2009).

In order to avoid the naïve effect, and consequently the static character of the simulations, the calibration scheme of the neural approaches was modified in this work. For this purpose, the ANNPI 1.0 software was programmed which integrates a graphical interface developed in Microsoft Visual Basic 6.0 with an independent calculation engine implemented in R 3.4.0 (Fig. 3) (Supplementary material). This configuration takes advantage of the full potential of both development tools. In this way, the classical calibration of the ANNs is carried out using the R package *neuralnet* (Fritsch et al., 2016), while the models evaluation as well as the automatic control of the variation of the parameters run by *neuralnet* is performed by ANNPI.

The *neuralnet* package developed by Fritsch et al. (2016) uses a classical calibration scheme that consists of stopping training when the global output error of the ANN is equal to or less than a user-determined threshold value. Usually high thresholds provide very fast convergences and bad goodness of fit in the validation phase due to a poor training. On the other hand, small thresholds imply very slow convergences and

mismatches in the model validation due to an overtraining effect.

To overcome these constraints, the ANNPI software drives to *neuralnet* through a script in which the user tests a range of errors thresholds as well as its decrement rate. In each calibration, at the end of each epoch, *neuralnet* checks if the global error is equal to or lower than the established threshold. If so, the script generates a weights file that is collected by ANNPI and that is used to calculate the Persistence Index (PI) (Kitanidis & Bras, 1980). ANNPI checks if the threshold of the last calibration corresponds to the user-determined minimum value. If not, a new threshold value is set and the control to *neuralnet* is returned. If the minimum threshold has been reached, ANNPI selects the neural structure where the best PI is obtained in the validation phase and saves the weights matrix (Fig. 3). Finally, the ANN selected is those that has the best performance within a pool of 30 repetitions (Iyer & Rhinehart, 1999; Antil & Rat, 2005).

The Persistence Index (PI), used in the ANNPI software for controlling the dynamic threshold in the calibration phase, is a function of the estimation lead-time for dynamical simulation models and can be defined by (Kitanidis & Bras, 1980):

$$PI = 1 - \frac{\sum_{i=1}^N (Q_t - \hat{Q}_t)^2}{\sum_{i=1}^N (Q_t - Q_{t-L})^2} \quad (1)$$

where Q_t is the observed discharge at the time step t ; Q_{t-L} is the observed discharge at the time step $t-L$; L is the estimation lead-time; \hat{Q}_t is the estimated discharge at the time step t and N is the total number of observations i of the validation set. When PI taking values equal to 1, there is a perfect adjustment between predicted and observed values. When PI is 0, the model has a naïve behaviour given as estimation the previous observation.

2.3. Alternative approaches to using ANNPI 1.0 for dynamical simulation of discharges

In the neural approaches evaluated, the autoregressive effect of the discharges of the immediately preceding month ($t-1$) and the variables in the month t of the medium precipitation and temperature and the 12-month SPI drought index SPI(12) were considered as independent variables using data series of the climatic stations located in the watersheds which discharge to the regulation reservoirs at study (Fig. 1). The dependent or output variable of the ANN was the inflow in month t at each of the regulation reservoirs analysed. The number of hidden layers tested ranged from 1 to 2 and the range of variation in the number of neurons per layer was between 3 and 15 neurons with increments of 2 units for each calibrated structure.

The inflow and air temperature data were used as monthly mean values and the precipitation data as monthly accumulated values. Long historical continuous observations of the discharges data series were used. For the Chanza reservoir from October 2002 to September 2012, for the Andévalo reservoir from January 2004 to September 2012, for the Beliche reservoir from November 1978 to September 1983, and for the Odeleite reservoir from July 1975 to September 1990. The inflows data to Spanish reservoirs (Chanza and Andévalo) were obtained from the Annual Reports of Gauging of the CEDEX (Centro de Estudios y Experimentación de Obras Públicas, Spanish Government, <https://ceh.cedex.es/anuarioaforos/default.asp>) and to Portuguese reservoirs (Beliche and Odeleite) from the Water Resources National Information System of Portugal (Sistema Nacional de Informação de Recursos Hídricos de Portugal SNIRH, <https://snirh.apambiente.pt/>). The precipitation and temperature data were provided of climatic stations of the Spanish State Meteorological Agency (Agencia Estatal de Meteorología de España AEMET, <https://www.aemet.es>) and of the Water Resources National Information System of Portugal (SNIRH) distributed over the study area (Fig. 1).

The data set of calibration for each reservoir was: Chanza reservoir from October 2002 to December 2009; Andévalo reservoir from January 2004 to December 2009; Beliche reservoir from November 1978 to December 1982; and Odeleite reservoir from July 1975 to December 1988. The data set of validation for each reservoir was: Chanza reservoir from January 2010 to September 2012; Andévalo reservoir from January 2010 to September 2012; Beliche reservoir from January 1983 to September 1983; and Odeleite reservoir from January 1989 to September 1990.

To assess the performance of the neural approaches during the validation phase, six accuracy measures were calculated: the coefficient of determination (r^2), the square root of the mean square error (RMSE), the mean absolute percentage error (MAPE), the Nash-Sutcliffe Efficiency coefficient (NSE), the Kling-Gupta Efficiency coefficient (KGE) and the persistence index (PI) (Kitanidis & Bras, 1980; Legates & McCabe, 1999; Pulido-Calvo & Portela, 2007; Gupta et al., 2009; Bayram & Çitakoğlu, 2023). These accuracy measures were calculated using Equations (1) to (5):

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^N (Q_i - \hat{Q}_i)^2}{N}} \quad (2)$$

$$\text{MAPE} = \frac{1}{N} \sum_{i=1}^N \left| \frac{\hat{Q}_i - Q_i}{Q_i} \right| \quad (3)$$

$$\text{NSE} = 1 - \frac{\sum_{i=1}^N (\hat{Q}_i - Q_i)^2}{\sum_{i=1}^N (Q_i - \bar{Q})^2} \quad (4)$$

$$\text{KGE} = 1 - \sqrt{(R-1)^2 + (\alpha-1)^2 + (\beta-1)^2} \quad (5)$$

where R is the Pearson's correlation coefficient ($r^2 = R^2$), α is the relationship between standard deviations of estimated and observed

discharges, β is the relationship between means of estimated and observed discharges and \bar{Q} is the mean of the discharges observed.

Additionally to determine the robustness model forecast, a Kruskal-Wallis test to examine statistical significant differences between observed and estimated discharges was carried out (Citakoglu & Demir, 2023; Coşkun & Citakoglu, 2023; Zouzou & Citakoglu, 2023). For that, Statistica 7.0 (StatSoft®) was used. All models were calibrated and validated in a CPU with a processor Intel® Core™ i7-4770 at 3.40 GHz and a graphic card NVIDIA GeForce® GTX760 with 4 MB memory.

3. Results and discussion

The goodness of fit in validation phase of the best neural models evaluated with the ANNPI 1.0 software are shown in Table 1. These neural models, calibrated for modelling inflows to Chanza, Andévalo and Odeleite reservoirs, showed good and very good performances in the validation phase, according to Bayram and Çitakoğlu (2023), with coefficients of determination (r^2) higher to 0.77, Nash-Sutcliffe Efficiency coefficients (NSE) higher to 0.75 and Kling-Gupta Efficiency coefficients (KGE) higher to 0.87. These satisfactory results were consistent with the Persistence Index (PI) values higher to 0.60. In the Beliche reservoir, the multi-criteria evaluation showed a worse performance based on KGE and PI values, although the neural approach performed well in remaining accurate measures (good and very good performance for r^2 and NSE, respectively, and reasonable prediction for MAPE) (Figs. 4 to 7). These results are a consequence, in part, of the capacity demonstrated by the ANNs to fit highly nonlinear functions and, on the other hand, of the novel training method proposed in this study. In all cases, the models had a high level of input parsimony with a maximum number of independent variables of four for to obtain results statistically satisfactory.

As for any neural network model, the main limitation of the developed method is determined by the time series length to inference and to predict. Since the models validation is done by predicting over a continuous time period not used during calibration, it is possible that the patterns variation contained in the calibration phase are not found in the validation period. This possibility is higher in those time series shorter and with a low variability, like it is the case of the Beliche reservoir in this study.

The results of neural approaches were compared with the simulations provided by the SIMPA model for the same validation periods (Table 1, Figs. 4 to 7). These simulations were obtained from web page of CEDEX (Centro de Estudios y Experimentación de Obras Públicas, Spanish Government, <https://www.miteco.gob.es/es/agua/temas/evaluacion-de-los-recursos-hidricos/evaluacion-recursos-hidricos-regimen-natural/>). The SIMPA (Integrated System for Rainfall-Runoff Modelling) is a conceptual and quasi-distributed model that simulates the process of transformation of precipitation into runoff in a natural regime, on a monthly scale, and in each of the cells in which the hydrographic region is reticulated. In this case, all the hydrographic region is gridded in square cells of 500 m on each side (CEDEX, 2020).

In the SIMPA simulations of the inflows to the regulation reservoirs of the Lower Guadiana Sub-basin, in some temporal periods, a displacement of one month between the observed and estimated discharges (naïve behaviour) were observed as well as an overestimation in some months characterised by high values of the discharges to reservoirs (Figs. 4 to 7). These effects were reflected in the very poor values of the Persistence Indexes (PI) (ranged between -1.97 to 0.16), the Nash-Sutcliffe Efficiency coefficients (NSE) (ranged between -0.72 to 0.26) and the Kling-Gupta Efficiency coefficients (KGE) (ranged between -0.03 to 0.50) (Table 1). This leads to a simplistic performance of the SIMPA model, at least in the some temporal periods of the hydrographic region analysed, even though the explained variances had acceptable statically values (r^2 higher to 0.44). This model produced a static map with a specific probability of streamflow occurrence that in some

Table 1

Goodness of fit in the validation phase of the best neural approaches that model the monthly inflows to the regulating reservoirs of the hydrographic region of the International Lower Guadiana River. Comparison with the SIMPA model and with a naïve model.

Reservoir	Model	r^2	RMSE (hm ³ /month)	MAPE (%)	NSE	KGE	PI
Andévalo (Spain)	Naïve	0.4088	20.01	59.94	0.2306	0.6204	0
	SIMPA	0.5508	11.67	64.94	0.2610	0.5030	-0.0819
	ANN (4 l-5 s-1 l)*	0.9544	2.79	17.11	0.9705	0.9295	0.9383
Chanza (Spain)	Naïve	0.5046	21.52	61.26	0.3783	0.6872	0
	SIMPA	0.5200	19.37	66.32	-0.7224	0.0658	-1.9714
	ANN (4 l-3 s-2 s-1 l)*	0.7799	7.11	39.00	0.7514	0.8706	0.6000
Odeleite (Portugal)	Naïve	0.2113	22.33	107.96	-0.0755	0.4594	0
	SIMPA	0.5731	20.42	62.45	0.1004	0.4896	0.1635
	ANN (3 l-5 s-1 l)**	0.9262	6.31	29.35	0.9140	0.8894	0.9174
Beliche (Portugal)	Naïve	0.2431	2.58	91.28	0.0080	0.4807	0
	SIMPA	0.4438	2.45	77.31	0.1085	-0.0328	0.1013
	ANN (3 l-5 s-1 l)**	0.7750	0.28	36.54	0.7716	0.4678	0.2010

Input or independent variables: *inflow to reservoir of the preceding month ($t-1$), medium precipitation and temperature in month t and the 12-month SPI drought index SPI(12) in month t ; **inflow to reservoir of the preceding month ($t-1$), medium precipitation in month t and the 12-month SPI drought index SPI(12) in month t .

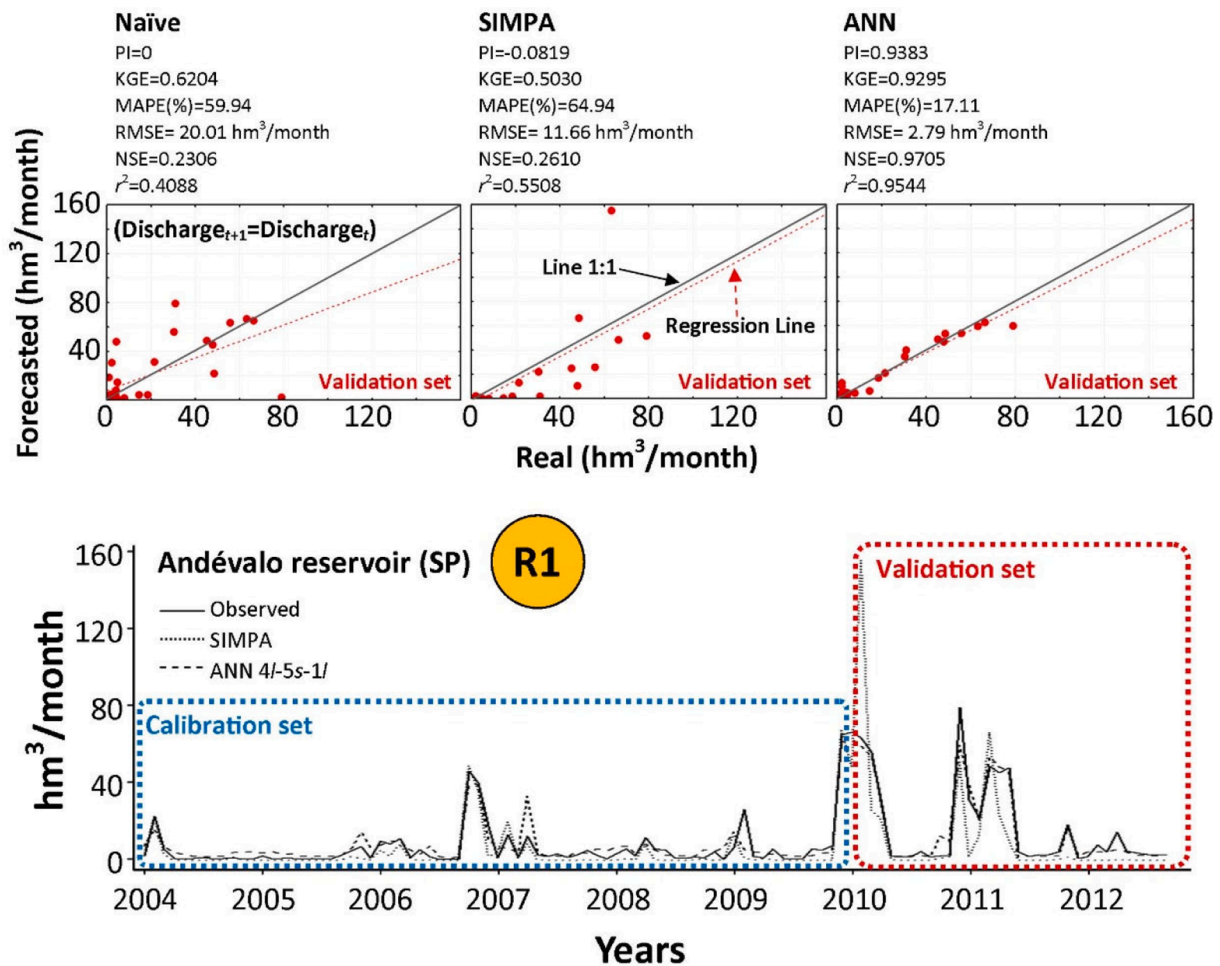


Fig. 4. Observed and estimated discharges by the neural approaches and SIMPA model in the Andévalo reservoir (SP = Spain, Fig. 1). The scatterplots and accuracy magnitudes of the naïve, SIMPA and ANN models in the validation periods are shown.

temporal periods, generally characterised by high values of the discharges to reservoirs, the monthly simulations are systematically very close to the discharges observed in the previous months. This performance reduces its applicability to facilitate near-real time predictions which is one of the main requirements for a decision-support system that can ensure reliable discharges information (Gastélum et al., 2009; Rajib et al., 2020).

Table 2 shows the results of the Kruskal-Wallis test for each model and reservoir between observed and estimated discharges in the

validation phase. In the Chanza and Andévalo reservoirs, the results indicate that observed and estimated values with the SIMPA model were from different distributions (medians of the data sets were significantly different). Instead, this behaviour was not detected for the Odeleite and Beliche reservoirs despite all accuracy measures in the validation phase were significantly better when the ANNs were used. This could be a consequence of the number of available data in the validation phase. Kruskal-Wallis test calculates the test statistic sorting the data into sets from the smallest to highest. This way, in time series with a low number

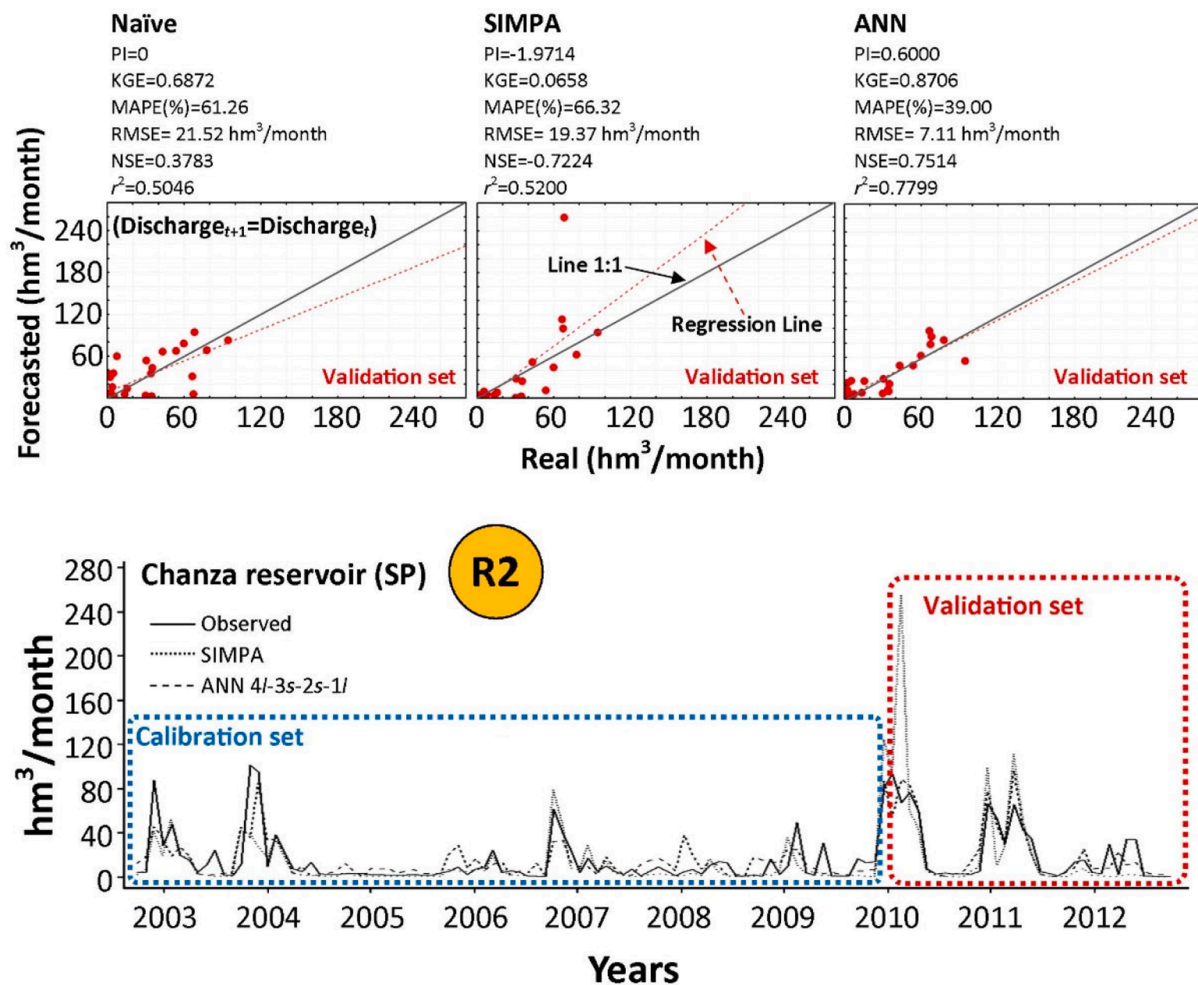


Fig. 5. Observed and estimated discharges by the neural approaches and SIMPA model in the Chanza reservoir (SP = Spain, Fig. 1). The scatterplots and accuracy magnitudes of the naïve, SIMPA and ANN models in the validation periods are shown.

of data (like Odeleite and Beliche reservoirs) a little change in the data distribution won't drive to reject H_0 .

The results obtained in this study show the capacity and potential of the software ANNPI 1.0 to be used for characterise and infer the temporary of the discharges regime in a specific hydrographic region using only a few catchment attributes as independent variables. This is due to the novel calibration scheme of the neural approaches proposed and developed in this study, which is based on a calibration procedure controlled by the Persistence Index (PI) that is function of the estimation lead-time, to allow to avoid the naïve effect (the estimation is the previous observation) and consequently the static character of the simulations.

Furthermore the SPI drought index, as independent variable, might be supporting the high goodness of fit obtained in the validation phase by the software ANNPI 1.0. It is well known that the selection of the independent variables involved in a phenomenon/process is one of the fundamental and critical stages for its modelling and, therefore, it conditions the characterisation, estimation and inference of the system under study (Bowden et al., 2005; Molotch et al., 2005; Li et al., 2022; Yin et al., 2022). Thus, the consideration of the characterisation and quantification of the drought temporal variability at a twelve-month scale (hydrological drought), by the SPI(12) index, seems to significantly condition the adaptive performance of ANNPI 1.0 as inference and forecast model of streamflow monthly regime in hydrographic basins with typical hot-summer Mediterranean climate conditions (Beck et al., 2018), which encourages the implementing water management adaptation measures to ensure its availability for different uses within a

decision horizon (Beça et al., 2023; Garrote et al., 2023).

In our study case, the Lower Guadiana Transboundary Basin, the developed approach for forecasting natural regime discharges could be implemented in simulations of reservoir water balances to assess the future water availability to ensure urban water supply, to improve the reliability of irrigation supply by providing the possible allocations according to the climatic conditions, and to guarantee the ecological flow requirements. To this end, several studies, such as Iglesias et al. (2011), Girard et al. (2015), Fabre et al. (2016) and Mereu et al. (2016), have evaluated water supply and demand management strategies, from which the importance of improving the dynamic modelling of water availability to find adaptive solutions is perceived, despite the associated uncertainty, for which the solution proposed in this work could be a very useful tool.

In this sense, in this hydrographic region, with a predominance of moderate and severe drought events that are repeated cyclically together with the increasing trend of irrigation water demand, the need to study and evaluate the current irrigation water requirements should be a priority in order to have clear and feasible governance and planning guidelines to carry out future actions to reduce irrigation deficits (such as cropping patterns and/or irrigation practices) in view of the expected expansion of irrigated area in the forthcoming years in southern Iberian Peninsula (Fader et al., 2016; Tocados-Franco et al., 2023).

The better estimations of the neural approximations in comparison with the SIMPA model could also be due to the fact that SIMPA is a model calibrated at a large scale (for the whole of peninsular Spain) with globally good results but that at a local scale (specific sub-basins) may

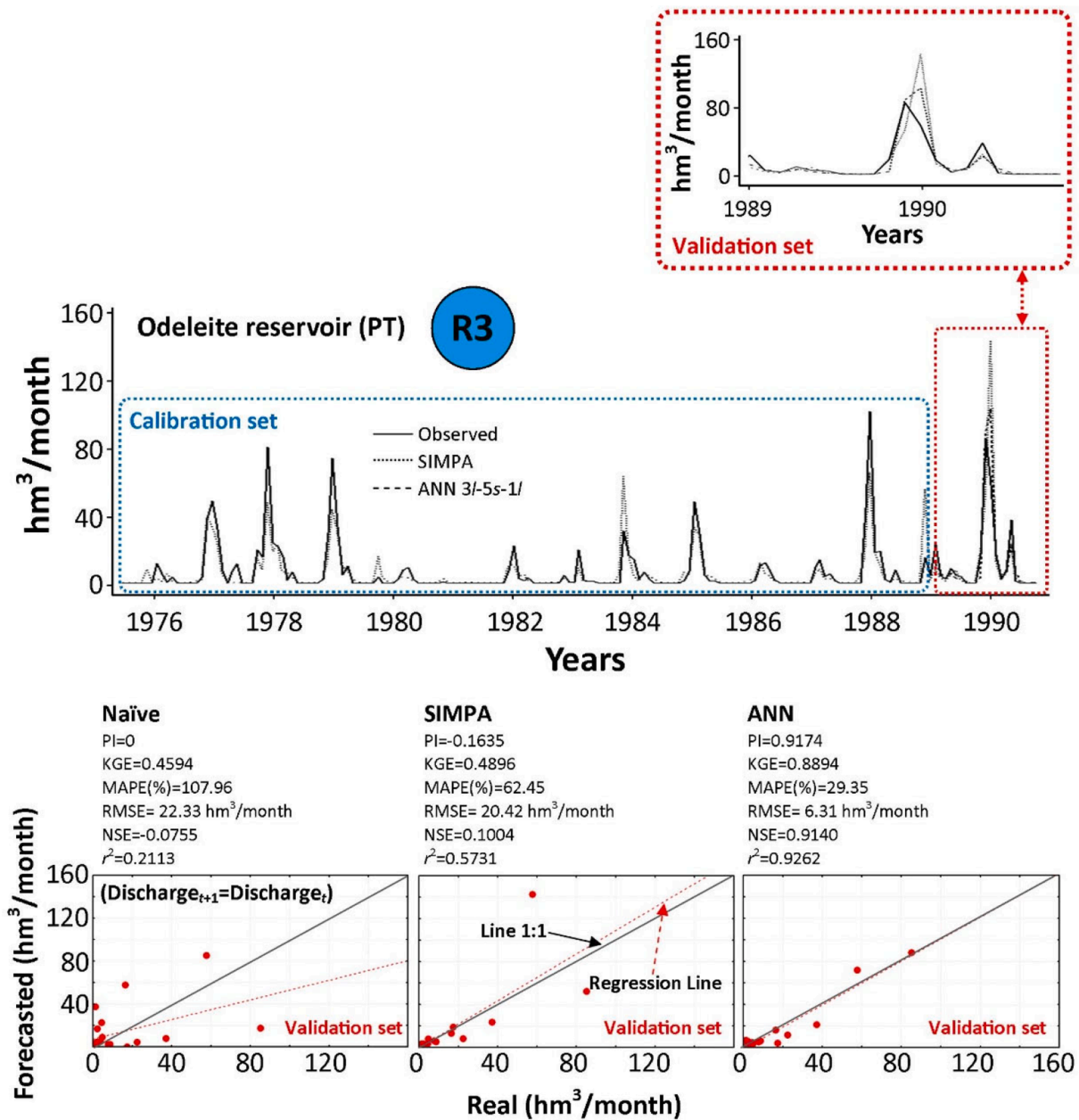


Fig. 6. Observed and estimated discharges by the neural approaches and SIMPA model in the Odeleite reservoir (PT = Portugal, Fig. 1). The scatterplots and accuracy magnitudes of the naïve, SIMPA and ANN models in the validation periods are shown.

present significant deviations with respect to the observed data (Cabezas, 2015). Therefore, it could be considered at the level of hydrological planning that the local heuristic modelling, that allows the inclusion of regionally variable knowledge, could be considered as a complementary tool to the SIMPA model in order to achieve greater reliability and consistency in the dynamic characterisation of the availability and compatibility of water resources. Nowadays, the coupling of models is an approach analysed to reduce the lack of geospecificity or ‘local relevance’ at large-scale streamflow modelling initiatives in order to achieve a better regional decision-support tool to facilitate operational management of river basins (Winsemius et al., 2013; Huang & Hattermann, 2018; Rajib et al., 2020).

4. Conclusions

The ANNPI 1.0 computer application has been designed and programmed considering a novel calibration procedure of the standard

back-propagation algorithm of neural approaches which is controlled by the Persistence Index (PI) depending of the estimation lead-time. Its application to the dynamical behaviour simulation of discharges monthly regime in the Lower Guadiana Transboundary Basin, with a high seasonal and interannual variability of precipitations, showed statistically very satisfactory performances when in the time series of streamflows in the calibration phase underlay the variation patterns of this water resources system. These results facilitating near-real time predictions which could help to improve the current management strategies and to take preventive and adaptive measurements for the balanced allocation of all uses and their compatibility with the environmental flows in the basin when it is subject to excessive water stress.

The integration of the long-term quantification of the temporal variability of drought, using the 12-month SPI index as an input variable to the neural approaches evaluated, seems to support the adaptive performance of ANNPI 1.0 as an inference and prediction model of the monthly streamflow regime in river basins characterised by the

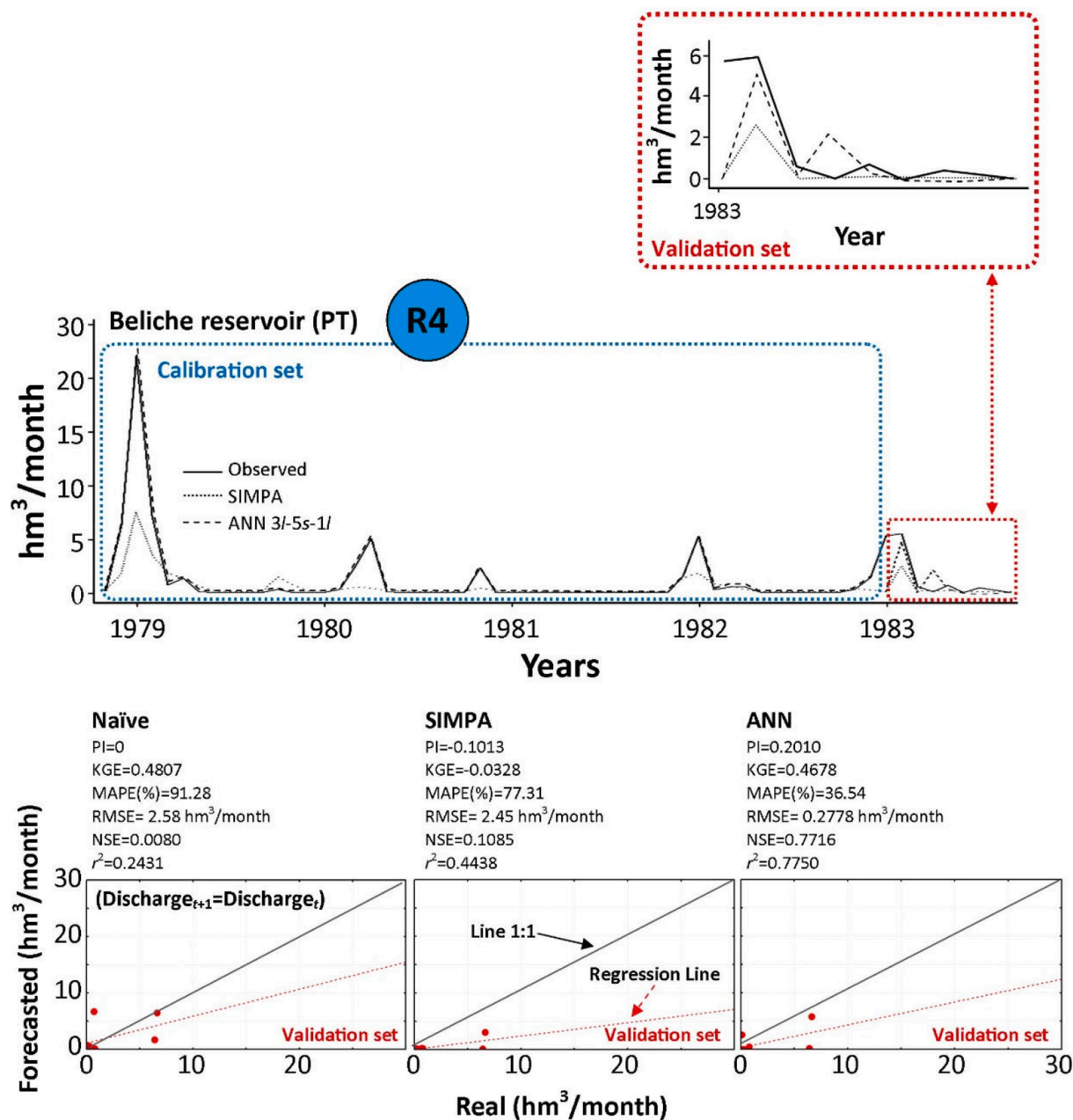


Fig. 7. Observed and estimated discharges by the neural approaches and SIMPA model in the Beliche reservoir (PT = Portugal, Fig. 1). The scatterplots and accuracy magnitudes of the naïve, SIMPA and ANN models in the validation periods are shown.

Table 2
Kruskal-Wallis (KW) test at 95% confidence level for observed and estimated values in the validation phase.

Reservoir	Model	Degree of freedom	KW statistic	p value	H ₀
Andévalo (Spain)	SIMPA	(1,66)	14.96	<0.001	Reject
	ANN (4 l-5 s-1 l)	(1,66)	0.3458	0.8525	Accepted
Chanza (Spain)	SIMPA	(1,66)	3.7749	0.0520	Reject
	ANN (4 l-3 s-2 s-1 l)	(1,66)	0.1336	0.7147	Accepted
Odeleite (Portugal)	SIMPA	(1,42)	0.1725	0.6779	Accepted
	ANN (3 l-5 s-1 l)	(1,42)	0.0040	0.9498	Accepted
Beliche (Portugal)	SIMPA	(1,18)	0.7125	0.3986	Accepted
	ANN (3 l-5 s-1 l)	(1,18)	1.6411	0.2002	Accepted

occurrence of moderate and severe drought events that repeat cyclically, which are common in hot-summer Mediterranean climate conditions.

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CRediT authorship contribution statement

Inmaculada Pulido-Calvo: Conceptualization, Formal analysis, Investigation, Methodology, Project administration, Software, Validation, Writing – original draft, Writing – review & editing. **Juan Carlos**

Gutiérrez-Estrada: Conceptualization, Formal analysis, Investigation, Methodology, Software, Validation, Writing – original draft, Writing – review & editing. **Víctor Sanz-Fernández:** Formal analysis, Investigation, Software, Writing – review & editing.

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.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.eswa.2024.123785>.

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